# **Subject Categories of the Division C. Chemistry and Materials**

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**Materials Processing** 

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Includes space-based development of products and processes for commercial application.

performance of thermally-throttled systems is presented. Uncertainties in modeling real-world thermal throttling systems are discussed. The possible use of thermal throttling characteristics as a means of propellant pressure regulation is also examined. DTIC

Electric Propulsion; Electrostatics; Ion Engines; Propellants; Throttling

19970020328 ERC, Inc., Tullahoma Operations Office, Tullahoma, TN USA

Design Study: Rocket Based MHD Generator Final Report, 6 May 1996 - 5 May 1997

May 1997; 76p; In English

Contract(s)/Grant(s): NASA Order H-13047D

Report No.(s): NASA-CR-204495; NAS 1.26:204495; ERC-R-97-017; No Copyright; Avail: CASI; A05, Hardcopy; A01, micro-

fiche

This report addresses the technical feasibility and design of a rocket based MHD generator using a sub-scale LOx/RP rocket motor. The design study was constrained by assuming the generator must function within the performance and structural limits of an existing magnet and by assuming realistic limits on (1) the axial electric field, (2) the Hall parameter, (3) current density, and (4) heat flux (given the criteria of heat sink operation). The major results of the work are summarized as follows: (1) A Faraday type of generator with rectangular cross section is designed to operate with a combustor pressure of 300 psi. Based on a magnetic field strength of 1.5 Tesla, the electrical power output from this generator is estimated to be 54.2 KW with potassium seed (weight fraction 3.74%) and 92 KW with cesium seed (weight fraction 9.66%). The former corresponds to a enthalpy extraction ratio of 2.36% while that for the latter is 4.16%; (2) A conceptual design of the Faraday MHD channel is proposed, based on a maximum operating time of 10 to 15 seconds. This concept utilizes a phenolic back wall for inserting the electrodes and inter-electrode insulators. Copper electrode and aluminum oxide insulator are suggested for this channel; and (3) A testing configuration for the subscale rocket based MHD system is proposed. An estimate of performance of an ideal rocket based MHD accelerator is performed. With a current density constraint of 5 Amps/cm(exp 2) and a conductivity of 30 Siemens/m, the push power density can be 250, 431, and 750 MW/m(sup 3) when the induced voltage uB have values of 5, 10, and 15 KV/m, respectively.

Derived from text

Magnetohydrodynamic Generators; Rocket Engines; Research Projects; Design Analysis; Faraday Effect; Magnets

# 23 CHEMISTRY AND MATERIALS (GENERAL)

19970019582 National Renewable Energy Lab., Golden, CO USA

Sixth workshop on the role of impurities and defects in silicon device processing

Tan, T., National Renewable Energy Lab., USA; Swanson, R., National Renewable Energy Lab., USA; Sopori, B., National Renewable Energy Lab., USA; Sep. 1996; 14p; In English; 6; Workshop on the Role of Impurities and Defects In Silicon Device Processing, 11 - 14 Aug. 1996, Snowmass, CO, USA

Contract(s)/Grant(s): DE-AC36-83CH-10093

Report No.(s): NREL/SP-413-21640; CONF-9608116-Summ.; DE96-013101; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The Sixth Workshop on the Role of Impurities and Defects in Silicon Device Processing was held in Snowmass Village, August 12-14, 1996. The workshop was attended by 87 participants from academic institutions and photovoltaic industry representatives, from the USA, Australia, Belgium, Canada, France, Germany, Italy, Japan, Belgium, and The Netherlands. The workshop consisted of nine sessions that addressed different aspects of impurities and defects in silicon and applications to solar-cell processing. Each session opened with some review talks summarizing recent advances in this field and introduced important issues for further discussions during a subsequent panel discussion session. In addition, the latest research results were presented in two poster sessions.

DOE

Conferences; Impurities; Crystal Defects; Fabrication; Solar Cells

19970019590 Virginia Polytechnic Inst. and State Univ., Dept. of Chemical Engineering, Blacksburg, VA USA Structure-Property Behavior of Organic-Inorganic Hybrid Materials Based on Sol Gel Chemistry *Final Report*, 1 Mar. 1994 - 31 Aug. 1996

Wilkes, Garth L., Virginia Polytechnic Inst. and State Univ., USA; Dec. 06, 1996; 95p; In English Contract(s)/Grant(s): F49620-94-I-0149; AF Proj. 2303

Report No.(s): AD-A320471; AFOSR-TR-97-0051; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

This work was directed at the synthesis and structure-property behavior of hybrid organic-inorganic network materials prepared by a sol gel reaction. Specific focus concerned the development of optically abrasion resistant coatings that could be utilized for both polymeric and metallic substrates. In the case of the latter, the purpose of the coating was to not only to supply abrasion resistance but, if possible, provide corrosion resistance as well. Considerable success was achieved in that several hybrid coatings were synthesized by reacting one or more metal alkoxides with functionalized organic moieties such as triethoxysilanated diethylene triamine (DETA) and related diamines or di or triol species. These functionalized organics, in conjunction with the alkoxide, were spin or dip coated on appropriate substrates and thermally cured. In some cases a primer molecule was also utilized to promote higher adhesion with the substrate the principal example being amino propyltrimethoxysilane. It has been demonstrated that the coatings display very good abrasion resistance for polymeric substrates, aluminum and copper but do not perform as well on steel or a phosphate coated steel. The final portion of the work concerned the development of porous inorganics made by the calcination of hybrid organic-inorganic network materials but where these networks were prepared by the use of functionalized polytetramethylene oxide oligomers of varied molecular weight that had been reacted with tetraethylorthosilicate (TEOS). It was demonstrated that calcination of these materials could lead to porous silicate powders possessing a specific surfaces near 1000 meters(exp 2)/gram. Furthermore, pore size characteristics of these powders were analyzed. It was concluded that such hybrid materials could serve as the base for developing highly porous powder materials for chromatography, catalyst

Sol-Gel Processes; Organic Materials; Inorganic Materials; Alkoxides; Abrasion Resistance; Coatings; Molecular Structure

19970019742 New Orleans Univ., Dept. of Chemistry, LA USA

Synthesis and Structure of 4-(4-Nitro-1,2,5-Oxadiazol-3-y1) -NNO-azoxyl-1,2,5-Oxadiazol-3-Amine

Zelenin, Alexander K., New Orleans Univ., USA; Stevens, Edwin D., New Orleans Univ., USA; Trudell, Mark L., New Orleans Univ., USA; Oct. 30, 1996; 16p; In English

Contract(s)/Grant(s): N00014-95-I-1339

Report No.(s): AD-A317707; TR-1; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The synthesis of the energetic compound 4-(4-NITRO-1,2,5-OXADIAZOL-3-YL)-NNO-azoxyl-1,2,5-oxadiazol-3-amine (3) was achieved in two steps from diaminofurazan (1). Compound 3 was characterized by X-ray diffraction. From the X-ray structure a bifurcated intramolecular H-bond between O(2)- H(2)- N(4) was observed. In addition, intramolecular H-bonding was observed between H(1) and N(7) of an adjacent molecule. One molecule of ethanol and one-half molecule of water per molecule of water of 3 was observed in the crystal lattice. However, no H-bonding was observed between the solvent molecules and 3 in the crystal lattice. Despite the presence of solvent in the crystal lattice, 3 was found to have a high crystal density (d = 1.856 g/cu cm).

**DTIC** 

Chemical Bonds; Crystal Lattices; Amines

19970019754 Missouri Univ., Columbia, MO USA

Growth and Microstructure of Protective Ceramic Films on Aluminum Final Report, 1 Aug. 1992 - 31 Jul. 1995

White, Henry W., Missouri Univ., USA; Sep. 29, 1996; 7p; In English

Contract(s)/Grant(s): DAAL03-92-G-0372

Report No.(s): AD-A316852; ARO-30134.1-MS-EPS; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The motivation for this collaborative work with T. Sugama and co-workers at Brookhaven National Laboratory is to develop a low temperature ceramic coating process suitable for aluminum and magnesium. Their method uses sol-precursor solutions with PolyGermanoSiloxane (PGS) or PolyTitanoSiloxane (PTS) additive. Crosslinked networks are formed by pyrolytic reactions near 350 C. The surface microstructure of these films were investigated by Raman spectroscopy, AFM, SEM and EDAX. AFM scans of a 30% TSPI, 20% PTS ceramic film on Al 6061 showed prominent cracks, indicating imperfect match of Al and ceramic film thermal expansion coefficients. Single element scans of the surface reveal highest levels of Al occurring in the cracks, as would be expected because the ceramic film is thinnest at the cracks. However, the ceramic film may not be zero in the cracks, and may afford some level of corrosion protection, if the crack is not too wide. These studies indicate that obtaining crack free films is difficult. Optical spectroscopy showed evidence for Si-O-Ge linkages, and for interfacial oxane bonding with the substrate in the PGS films.

**DTIC** 

Aluminum; Protective Coatings; Ceramic Coatings

19970019946 Defence and Civil Inst. of Environmental Medicine, North York, Ontario Canada

# A Comparison Measurement of the Physical Properties of Round-Robin Test Materials

Cain, Brad, Defence and Civil Inst. of Environmental Medicine, Canada; Oct. 1996; 13p; In English

Report No.(s): AD-A320403; DCIEM-96-TM-64; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

A round-robin test of procedures for assessing certain textile properties has been proposed as part of a TTCP-PTP3 effort to facilitate the exchange of data between countries using different apparatuses. The objective of that study, Operating Assignment 9, is to determine whether values of thermal conductivity and water-vapour permeability of various fabrics are comparable when measured on two different apparatuses: the CORD Sweating Hot Plate (used by Australia and Canada) and the Hoenstein Sweating Hot Plate (used by the UK and the USA). Several fabric samples were submitted for independent testing by various nations. Sweating hot plates were developed as research tools to examine questions of combined heat and moisture transport through clothing ensembles rather than as an apparatus for determining fabric characteristics. As such, there was some concern that the material property values obtained with a sweating hot plate may not be sufficiently precise. The work presented here is an alternative measure to the sweating hot plate approach for determining the relevant material properties. The two apparatuses used in this investigation were specifically designed to measure thermal conductivity and water-vapour permeability and should thus provide an accurate benchmark for comparison of the other methods. As this is an interim report, no comparison was done of the results obtained to sweating hot plate values.

DTIC

Permeability; Perspiration; Textiles; Thermal Conductivity; Water Vapor; Fabrics

19970019955 Edgewood Research Development and Engineering Center, Research and Technology Directorate, Aberdeen Proving Ground, MD USA

#### Hydrolysis of HT to Biodegradable Products Final Report, Mar. - Sep. 1996

Harvey, Steven P., Edgewood Research Development and Engineering Center, USA; Szafraniec, Linda L., Edgewood Research Development and Engineering Center, USA; Beaudry, William T., Edgewood Research Development and Engineering Center, USA; Rohrbaugh, Dennis K., Edgewood Research Development and Engineering Center, USA; Dec. 1996; 23p; In English Report No.(s): AD-A320295; ERDEC-TR-376; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

HT is a powerful vesicant which was produced for use as a chemical warfare agent. The agent is a mixture of 60 wt% 2,2'-dichlorodiethyl sulfide ('HD' or 'sulfur mustard') and 40 wt% bis-(2-(2-chloroethylthio) ethyl) ether (T). HT reacts with water to form primarily thiodiglycol (TDG) and bis-(2-(2-hydroxyethylthio) ethyl) ether (T-OH). TDG has very low toxicity and is known to be biodegradable, whereas the toxicity and biodegradability of T-OH are unknown. For these reasons, the acidic hydrolysis of T-OH to TDG was investigated in the presence of HCl alone (resulting from the initial T hydrolysis) and HCl amended with equimolar amounts of HBr and HI. In the presence of HCl alone, TDG formation was relatively slow, whereas HBr and HI enhanced the rate of conversion of T-OH to TDG. The hydrolysis conditions studied were selected to be consistent with a subsequent biological treatment, and results suggest an approach for a combined hydrolysis/biodegradation process for HT, similar to one previously investigated for HD.

DTIC

Hydrolysis; Chemical Warfare; Biodegradation

19970019964 European Space Agency. European Space Research and Technology Center, ESTEC, Noordwijk, Netherlands Verification of the Baking Efficiency Using Micro-VCM Test Data

Zwaal, A., European Space Agency. European Space Research and Technology Center, ESTEC, Netherlands; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 41-49; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Baking of spacecraft materials and/or spacecraft hardware is often done in order to reduce the risk of contamination of critical items by outgassing species. The baking parameters are often cost-effectively selected and the efficiency of the baking is unknown. Normal material selection criteria, i.e. 1.0 % TML and 0.10 % CVCM, according to the Micro-VCM test as per specification ESA-PSS-01-702 do not guarantee clean spacecraft. Initial harder requirements as a CVCM of 0.01 % were practically not feasible because of limitations in the detection limits. For contamination critical (e.g. optical) components in spacecraft and for items in the vicinity of critical elements, it is recommended to select materials, of which the contamination potential is low or can be lowered by baking. This recommendation is even more valid in case solar radiation is involved: lessons learned from the returned LDEF, STSA and EURECA are that outgassed contaminants can be 'frozen' when solar radiation is involved. Baking of materials or hardware will reduce the contamination potential and will result in a lower contamination of the spacecraft in orbit. Nowadays baking of structural parts, multilayer insulation and harness is more or less becoming standard for contamination critical spacecraft as e.g. SOHO. The efficiency of the materials baking can however be measured using the Micro-VCM outgassing tests on unbaked

and on similar baked materials. Two successive Micro-VCM tests on the same sample were performed and gave information on thermal degradation effects and on the lowest achievable contamination potential. This paper describes the effect of baking on the contamination potentials of materials and for this description, outgassing data of the Micro-VCM tests are used as a baseline. Author

Spacecraft Contamination; Baking; Outgassing; Thermal Degradation; Spacecraft Components; Residual Gas

# 24 COMPOSITE MATERIALS

Includes physical, chemical, and mechanical properties of laminates and other composite materials. For ceramic materials see 27 Nonmetallic Materials.

19970019349 Instituto Nacional de Pesaciais Espaciais, Sao Jose dos Campos, Brazil

# Optimization of Nonhomogeneous Facesheets in Composite Sandwich Plates

Filho, Mario Kataoka, Toronto Univ., Canada; 1997; 202p; In English

Report No.(s): INPE-6139-TAE/024; Copyright; Avail: Issuing Activity (Inst. Nacional de Pesquisas Espaciais, Caixa Postal 515, Sao Jose dos Campos, Brazil), Hardcopy, microfiche

Minimum weight design is an important criterion in aircraft and spacecraft because it allows either an increased payload or higher performance. As a result, the use of composite sandwich panels has grown due to their light weight and high rigidity. In order to further increase the efficiency of these structures, designers have used different materials in different shapes in the facesheets and in the core. One of the most recent innovations has been the use of a uniform net of carbon fibre/epoxy as the facesheets. In the present study, the optimal design of sandwich plates with heterogeneous face-sheets is treated. The plate mass is minimized, considering the first natural frequency and certain failure loads as constraints. Weight reduction is obtained by defining a nonuniform distribution of composite material in the facesheets. Initially, the facesheets are assumed to be constructed of composite strips in a regular pattern. During the optimization process, both the widths of the strips and the spacing between them are varied to decrease the amount of material used. Such a design is conceptually straightforward to manufacture and, therefore, would lead to improved performance with little cost penalty. In order to solve this problem, it is first necessary to develop a computer code to determine the natural frequencies and the stresses in these plates. The bending and vibration problems for sandwich plates with heterogeneous facesheets are solved using the Ritz Method in conjunction with the assumptions formulated by Reissner for sandwich plates. Since the sandwich plate considered has facesheets constructed of nets and the computer code was developed to analyze laminates with heterogeneous continuous layers, it was necessary to use a procedure to approximate the nonuniform net as a smoothed orthotropic heterogeneous continuum. The smoothing process is accomplished using the theory of homogenization and the material coefficients were calculated using the Finite Element Method. Two approaches were considered to define the design variables of the problem: an independent design approach, in which the facesheets are discretized into regions with uniform design parameters; and a reduced basis formulation, in which the design is specified by a linear combination of orthogonal basis functions. It has been demonstrated that variation in density is important and can lead to significant design improvement. Across of the face of the optimally designed plate, the density varies by a factor of 9. Also, the problems solved showed that the mass of the facesheets can be reduced up to 50%.

Author

Composite Structures; Sandwich Structures; Plates (Structural Members); Fiber Composites; Epoxy Matrix Composites; Carbon Fibers

19970019653 Hughes Technical Center, Atlantic City International Airport, NJ USA

# **Bolted Joints in Composite Structures: An Overview**

Oplinger, D. W., Hughes Technical Center, USA; AGARD Conference Proceeding: Bolted/Bonded Joints in Polymeric Composites; Jan. 1997; 12p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A03, Hardcopy; A03, microfiche

Investigations of bolted joints from the introduction of advanced composites in the mid-to-late 1960's to the present are reviewed. Numerous efforts aimed at applying two dimensional elastic stress analysis in conjunction with appropriate testing have been conducted. Modelling of the pinplate contact problem by a radial displacement condition rather than a radial pressure distribution is physically more realistic and has been done in a number of efforts, starting with that of Oplinger and Gandhi in the early 1970's. However in the case of the problem of bearing-bypass stress interaction which is in principle controlled by the radial displacement description of the contact problem, a number of efforts have provided useful results, especially in conjunction with adjustments based on test data by superposition of the half-cosine radial pressure distribution for pure bolt bearing load and the

open-hole plate solution for bypass load. Approaches to predicting failure using results of 2-D elasticity analysis are discussed. In addition, recent effort addressing bearing failure on the basis of the three dimensional stress state is considered. Currently, the details of the three-dimensional contact problem associated with bending deflections of the fastener as well as the interaction of the fastener head with the surfaces of the joint plate elements are seen to need additional study.

Bolted Joints; Composite Structures; Composite Materials; Elastic Properties; Stress Analysis; Bolts

# 19970019654 National Research Council of Canada, Institute for Aerospace Research, Ottawa, Ontario Canada Bolted Joint Technology in Composite Structures: Analytical Tools Development

Poon, C., National Research Council of Canada, Canada; Xiong, Y., National Research Council of Canada, Canada; Bolted/Bonded Joints in Polymeric Composites; Jan. 1997; 12p; In English; Also announced as 19970019652

Contract(s)/Grant(s): DNDFE-220794NRC08; NCR Proj. 3G3; Copyright Waived; Avail: CASI; A03, Hardcopy; A03, microfiche

Graphite fiber reinforced polymeric composites have been used extensively in the primary and secondary structures of modern military and civilian aircraft. In these structures, bolted joints are important considerations in structural design and repair. Reviews of the literature indicated that most of the current design methods were developed for single fastener Joints and, in general, design optimization, three dimensional effects and fatigue behaviour required further research and development. This paper reviews the results of the bolted joint technology development project sponsored by the Institute for Aerospace Research and the Canadian Department of National Defence. The project includes the development of computer-aided design tools for optimizing the design of multi-fastener composite joints and for predicting the fatigue behavior of pin/bolt loaded composite laminates. Current focus and future direction of the development of analytical tools for repair of composite structures and other applications are presented.

Author

Bolted Joints; Composite Structures; Fiber Composites; Fasteners; Graphite; Laminates; Bolts

#### 19970019655 Wright Lab., WL/FIBAD, Wright-Patterson AFB, OH USA

#### A Review of Composite Joint Analysis Programs

Venkayya, V. B., Wright Lab., USA; Tischler, V. A., Wright Lab., USA; AGARD Conference Proceeding: Bolted/Bonded Joints in Polymeric Composites; Jan. 1997; 20p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A03, Hardcopy; A03, microfiche

Several joint analysis programs funded by U.S. government agencies during the 1970s, 1980s and 1990s were reviewed. The review covered bolted, bonded, bolted-bonded and repair programs. In a few cases the results obtained from these programs are compared. A number of related references were cited for the purpose of obtaining additional details.

Bolted Joints; Bolts; Laminates; Composite Materials

# 19970019664 Defence Research Agency, Structural Materials Center, Farnborough, UK Surface Treatment and Bonding of Thermoplastic Composites

Shaw, S. J., Defence Research Agency, UK; Comyn, J., Defence Research Agency, UK; Mascia, L., Loughborough Univ. of Technology, UK; Jan. 1997; 12p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A03, Hardcopy; A03, microfiche

The use of structural adhesives in engineering applications can offer substantial benefits in comparison to more traditional joining techniques such as mechanical fastening and welding. These include: Improved fatigue performance; ability to join dissimilar materials; ability to join thin gauge materials and honeycomb constructions; and simpler and cheaper component construction. Operational benefits which can result from the significant use of bonding include improved equipment performance, resulting largely from the significant weight reductions which adhesive bonding can provide, together with substantial reductions in both procurement and life-cycle maintenance costs. In particular, the use of adhesive bonding in the construction of advanced lightweight composite structures will be of major importance since mechanical fastening would impose penalties in terms of mechanical integrity and weight.

Derived from text

Adhesive Bonding; Thermoplasticity; Honeycomb Structures

# 19970019665 Politecnico di Milano, Dept. di Ingegneria Aerospaziale, Milan, Italy Hygrothermal Fatigue of Composite Bonded Joints

Giavotto, V., Politecnico di Milano, Italy; Caprile, C., Politecnico di Milano, Italy; Sala, G., Politecnico di Milano, Italy; Jan. 1997; 10p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A02, Hardcopy; A03, microfiche

Adhesive bonding is the optimal technique to join composite laminates, because it does not induce stress concentrations, fibres cutting, resin delaminations and problems due to electrochemical non-compatibility. Notwithstanding, in many cases bolted and riveted joints have to be used, mainly in hot-wet environmental conditions, as well as when composites have to face chemically aggressive fluids, as hydraulic and de-icing fluids, oils and fuels. Moreover, the influence exerted on bonded joints by technological defects (voids, inclusions) and barely visible damages (due to low-energy impacts) should be addressed. The results of a research on the fatigue behaviour of wet-conditioned, impacted and defective composite bonded joints are reported. Single and double lap geometry carbon fabric/epoxy joints are considered. bonded with high-toughness adhesive. The specimens were wetconditioned in hot water (70 C) up to saturation. Barely visible damages were produced in the bonded region (influencing both the composite adherents and the adhesive layer) by means of low-energy impacts (0.5 J per mm laminate thickness) imparted by a spring-propelled horizontal apparatus with 20 mm hemispherical steel impactor). Defective bondings were simulated by including copper inserts, located in different positions. Defective, impacted and wet conditioned specimens were subjected to static and constant amplitude fatigue testing (tension-compression, R=1, 6Hz frequency); their performances were compared to the behaviour of plain specimens. The stiffness decrease and the damage growth were continuously monitored during the testing by means of extensometers and NDI techniques (ultrasonic scanning and dye penetrant radiography). The results consist in the comparison of the static stress-strain curves relevant to plain, defective, impacted and wet-conditioned specimens, the curves of stiffness decrease vs. number of cycles and the Woehler curves. Finally, the static characteristics and the fatigue performances are correlated with the damage growth and the adhesive progressive degeneration by analysing the radiographs and the SEM micrographs of the failed bonded region, in order to propose an interpretative model. Author

Bonded Joints; Bolted Joints; Adhesive Bonding; Adhesives; Laminates; Stress-Strain Relationships; Riveted Joints; Resins; Hygral Properties

# 19970019667 Northrop Grumman Corp., Military Aircraft Systms Div., Pico Rivera, CA USA

# Attachment of Ceramic Matrix Composites of AFR700B Composites for Exhaust Washed Airframe Structures

Atmur, Steven, Northrop Grumman Corp., USA; Colby, Mary, Northrop Grumman Corp., USA; Tomasek, Mary, Northrop Grumman Corp., USA; Hagen, Michael, Northrop Grumman Corp., USA; Sherrill, David, Northrop Grumman Corp., USA; Foreman, Charles, Northrop Grumman Corp., USA; Dolvin, Douglas, Wright Lab., USA; Jan. 1997; 10p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A02, Hardcopy; A03, microfiche

Current industry practice separates the design of an air vehicle's propulsion system from the design of its airframe. This practice causes many problems and inefficiencies particularily for advanced exhaust nozzle designs. It results in redundant aircraft structure to be insulated and shielded from the engine thermal and acoustic emanations. Perhaps, most importantly, it causes buckling and cracking at the joint interfaces where the thermally induced stresses are reacted. The critical joint interfaces are the cocured/bonded joints between layers of dissimilar materials and the mechanical joints between structural components. Northrop Grumman's concept is to modernize the design, analysis, and construction of future high performance aircraft by integrating the exhaust nozzle/ exhaust washed structural components into the primary airframe structure through a combination of organic and ceramic matrix composite materials. Designing bolted and bonded joints to carry induced loads efficiently, then, is critical to an integrated structural approach. Northrop Grumman has evolved a variety of approaches to transfer loads, including co-bonding of dissimilar materials and unique joint designs. Ceramic matrix composite/ AFR700B bolted and bonded joints have been identified as a critical need, and under Air Force-contracted research, joints have been designed and analyzed and will be fabricated. Sub-element testing, including static and fatigue, will validate the design and analytical methodologies. Durability and maintainability will be validated through testing and nondestructive evaluation. Trade-off analysis performed on the bolted and bonded joints will address structural efficiency, reliability, supportability, and battle damage tolerance.

Author

Ceramic Matrix Composites; Bolted Joints; Bonded Joints; Insulation; Laminates; Structural Design; Systems Engineering; Temperature Effects

# 19970019668 Lockheed Martin Tactical Aircraft Systems, Fort Worth, TX USA

#### 3-D Composites in Primary Aircraft Structure Joints

Bersuch, Larry, Lockheed Martin Tactical Aircraft Systems, USA; Hunten, Keith, Lockheed Martin Tactical Aircraft Systems, USA; Baron, Bill, Wright Lab., USA; Tuss, James, Wright Lab., USA; Jan. 1997; 10p; In English; Also announced as

19970019652; Copyright Waived; Avail: CASI; A02, Hardcopy; A03, microfiche

Three-dimensional woven and braided inserts and preforms, when cocured into primary wing and fuselage laminate structure, offer reduced weight, increased performance, lower costs, and improved damage tolerance and ballistic survivability for future aircraft. to achieve these benefits, three-dimensional (3-D) weaving and braiding technologies must be characterized through the development of design criteria, design methods, structural concepts, and manufacturing processes. In addition to 3-D weaving and braiding, z-direction reinforcement can be achieved through in-process fiber insertion with processes such as z-spiking, stitching, and short fiber additions to adhesives. Innovative applications of these technologies, combined with net shape curing processes such as resin transfer molding (RTM), electron beam cure, diaphragm forming, fiber placement, and cocuring, will result in the elimination of machined metal load fittings, fasteners, and reduction in weight at composite joints on future aircraft. Wing applications for 3-D composites would be at the intersection of spars and ribs and in the radius area between spars/ribs and the lower skin of a cocured wing assembly. In fuselage structure, 3-D composites eliminate the need for machined fittings and fasteners at concentrated load joints such as those at inlet duct, weapons bay, gun-trough, and fuel floor intersections with bulkheads/frames. This paper is directed at design for manufacturing of 3-D composite structures to best exploit the structural properties that they exhibit.

Author

Aircraft Structures; Composite Materials; Composite Structures; Curing; Fuselages; Laminates; Resin Transfer Molding; Wings; Three Dimensional Composites; Structural Design

#### 19970019669 Aztex, Inc., Waltham, MA USA

#### **Z-Fiber Technology and Products for Enhancing Composite Design**

Freitas, G., Aztex, Inc., USA; Fusco, T., Aztex, Inc., USA; Campbell, T., Foster-Miller Associates, Inc., USA; Harris, J., Foster-Miller Associates, Inc., USA; Rosenberg, S., Foster-Miller Associates, Inc., USA; Jan. 1997; 8p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A02, Hardcopy; A03, microfiche

Z-Fiber(TM) technology uses small, solid, cylindrical pins to greatly enhance the performance of composite structures. These pins, typically 0.25 to 0.50 mm in diameter, can be used for many structural applications. Z-Fibers, either composite or metal, are inserted through the thickness of a composite laminate to increase out-of-plane strength, damage resistance, and through thickness thermal conductivity. Z-Fiber is also used for structural joints and can be designed to be the structural network of the core material in an extremely weight and cost efficient sandwich structure. Z-Fiber technology has been under development for over ten years. The growth of this technology, originally developed by Foster-Miller Inc., has begun to move at a very accelerated rate under Aztex Inc. during the past two years. Despite this extended development period, the revolutionary advances in the performance of composite structures made possible by this technology are only now becoming fully apparent. When used at the conceptual stage of aircraft design, when the overall structural arrangement is being formulated, Z-Fiber technology can completely change the current design approaches. This paper presents a general overview of Z-Fiber technology and products and focuses on the work to date to form structural joints. The paper demonstrates, even at this early stage of development, Z-Fiber's capability to outperform fasteners and significantly increase the static survivability of composites.

Composite Structures; Aircraft Design; Thermal Conductivity; Structural Design; Sandwich Structures; Laminates

#### 19970019689 International Business Machines Corp., Endicott, NY USA

#### IBM, Endicott second year annual report. Executive summary Annual Report

Gaynes, M.A., International Business Machines Corp., USA; [1996]; 34p; In English; Limited Reproducibility: More than 20% of this document may be affected by micriofiche quality

Contract(s)/Grant(s): DE-FC04-94AL-98817

Report No.(s): DOE/AL/98817-8-Pt.2; DE97-000847; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

PMSP (Polymer Metal Solvent Paste) material must be deposited on a five inch wafer with 100% bump survival. The target geometry is 0.010(double prime) diameter, and 0.004(double prime) high with a flat surface. Accomplishments: The photobumping process has been refined to yield bumps that are 0.010 'in diameter and greater than 0.0035' high. The surface is flat and bonding results in a strong bond with no air entrapment between the chip bump and card pad. Initial work with photobumping yielded a bump surface that was concave. In photobumping, 0.004(double prime) thick photoresist is imaged to create apertures. These apertures are filled with PMSP in two passes with a solvent drying process that occurs between the first and the second pass After the first pass filling, solvent from the PM SP interacted with the photoresist and caused the top surface, at the circumference of the aperture, to shrink. On the second pass filling, this slightly depressed surface fills up with PM SP. We call this blooming because the diameter of the bump is extended at the surface. When the photoresist is stripped, the thin surface extension of the bump diameter of the bump is extended at the surface.

ter is folded over on top of the bump. This fold created a ridge at the circumference of the bump that would make initial contact with the card surface during bonding. The result was a high probability of air entrapment at the joint interface. The blooming problem was corrected by changing from an aqueous to a semiaqueous photorcsist that was more solvent resistant. Flat surface bumps are made with 100% yield on five inch wafers. Double layers of 0.002(double prime) photoresist are used to define the nearly 0.004(double prime) high bumps. Work is in progress to use single layers of 0.003(double prime) and 0.004(double prime) photoresist. A single layer should eliminate perturbations from a straight side wall profile that exist near the interface of a double photoresist layup.

DOE

Bonding; Wafers; Joints (Junctions); Polymer Matrix Composites; Polymeric Films; Pastes

19970019694 Cornell Univ., Dept. of Materials Science and Engineering, Ithaca, NY USA

Atomic Mechanisms of Flow and Fracture at Metal-Ceramic Interfaces and their Role in the Design of Metal Matrix Composites *Final Report*, 15 May 1993 - 14 May 1996

Raj, Rishi, Cornell Univ., USA; Nov. 05, 1996; 25p; In English

Contract(s)/Grant(s): F49620-93-1-0228

Report No.(s): AD-A319998; AF-AFOSR-TR-0044-97; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

This report describes new and significant results that can be applied in the microstructure design for optimum mechanical performance of metal-ceramic composites and laminates. There are three elements to these recommendations: (1) the design of the atomic structure of metal-ceramic interfaces, (2) identification of the critical length scale in the two phase microstructure, and (3) prediction of the microstructural conditions under which the thermal conductivity of the composite becomes significantly influenced by the thermal boundary resistance of interfaces. In the first topic we show that the beneficial effect of titanium interlayers at a copper/alumina interface is accomplished with only about one monolayer; with further increase in the titanium interlayer thickness having an insignificant effect on the interfacial strength. In the second topic we show that the metal ligament size is the key microstructural parameter in controlling the flow stress, the fracture stress and the fracture toughness of metal-ceramic composites. The metal ligament size is important because dislocation activity in the metal, which produces pile ups against the interface, is the critical event in flow and fracture of composites. In the third area we show that the interfacial thermal boundary resistance plays a dominant role in the overall thermal conductivity of the composite when the microstructural scale becomes smaller than about 1 micro m.

DTIC

Metal Matrix Composites; Fractures (Materials); Laminates; Ceramic Matrix Composites; Plastic Deformation; Stress Analysis; Aluminum Alloys; Copper Alloys; Fracture Strength

19970019933 Sandia National Labs., Albuquerque, NM USA

### Damage in unidirectional graphite/epoxy laminates containing a circular hole

Yang, Fan, Michigan Univ., USA; Chow, C. L., Michigan Univ., USA; Fang, H. Eliot, Sandia National Labs., USA; 1996; 9p; In English; Mechanical Engineering Congress and Exhibition, 17-22 Nov. 1996, Atlanta, GA, USA

Contract(s)/Grant(s): DE-AC04-94AL-85000

Report No.(s): SAND-96-2323C; CONF-961105-12; DE96-015190; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

In this paper, a damage mechanics model is described for determining progressive damage processes in unidirectional graphite/epoxy composite plates containing a central hole subjected to off-axis uniaxial tension. The inelastic behavior of these composite materials is attributed to the irreversible thermodynamics processes involving energy dissipation and stiffness variation caused by damage initiation and accumulation. The mechanical response of the composites is investigated by using a nonlinear finite element procedure formulated with a set of damage coupled constitutive equations. Separate damage criteria are derived for fiber failure and for matrix or fiber/matrix interaction failure in unidirectional composites. Validation of the damage model is achieved by comparing the numerical prediction and experimental data obtained from a Moire interferometry technique. It has been found that failure of the composite material near the hole region takes the form of an extensive damage zone. The macrocrack initiates at the material point near the hole boundary with a high damage value and propagates along the direction of damage zone extension. Preliminary results indicate that the proposed damage model is an effective method of studying progressive failure behavior of unidirectional composite laminates containing a circular hole and can be readily extended to examine the damage response of composite structures.

DOE

Graphite-Epoxy Composites; Composite Structures; Plates (Structural Members); Holes (Mechanics); Crack Initiation; Finite Element Method; Crack Propagation; Damage Assessment; Laminates

19970020046 NASA Lewis Research Center, Cleveland, OH USA

# Probabilistic Micromechanics and Macromechanics for Ceramic Matrix Composites

Murthy, Pappu L. N., NASA Lewis Research Center, USA; Mital, Subodh K., Toledo Univ., USA; Shah, Ashwin R., NYMA, Inc., USA; Jun. 1997; 16p; In English

Contract(s)/Grant(s): NAS3-27186; RTOP 505-63-12

Report No.(s): NASA-TM-4766; NAS 1.15:4766; E-10485; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The properties of ceramic matrix composites (CMC's) are known to display a considerable amount of scatter due to variations in fiber/matrix properties, interphase properties, interphase bonding, amount of matrix voids, and many geometry- or fabrication-related parameters, such as ply thickness and ply orientation. This paper summarizes preliminary studies in which formal probabilistic descriptions of the material-behavior- and fabrication-related parameters were incorporated into micromechanics and macromechanics for CMC'S. In this process two existing methodologies, namely CMC micromechanics and macromechanics analysis and a fast probability integration (FPI) technique are synergistically coupled to obtain the probabilistic composite behavior or response. Preliminary results in the form of cumulative probability distributions and information on the probability sensitivities of the response to primitive variables for a unidirectional silicon carbide/reaction-bonded silicon nitride (SiC/RBSN) CMC are presented. The cumulative distribution functions are computed for composite moduli, thermal expansion coefficients, thermal conductivities, and longitudinal tensile strength at room temperature. The variations in the constituent properties that directly affect these composite properties are accounted for via assumed probabilistic distributions. Collectively, the results show that the present technique provides valuable information about the composite properties and sensitivity factors, which is useful to design or test engineers. Furthermore, the present methodology is computationally more efficient than a standard Monte-Carlo simulation technique; and the agreement between the two solutions is excellent, as shown via select examples.

Author

Ceramic Matrix Composites; Micromechanics; Fiber-Matrix Interfaces; Ply Orientation; Probability Theory; Fabrication; Matrix Materials

#### 19970020059 NASA Lewis Research Center, Cleveland, OH USA

#### Two-Flux Green's Function Analysis for Transient Spectral Radiation in a Composite

Siegel, Robert, NASA Lewis Research Center, USA; Journal of Thermophysics and Heat Transfer; Dec. 1996; Volume 10, No. 4, pp. 681-688; In English

Report No.(s): NASA-TM-112841; NAS 1.15:112841; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

An analysis is developed for obtaining transient temperatures in a two-layer semitransparent composite with spectrally dependent properties. Each external boundary of the composite is subjected to radiation and convection. The two-flux radiative transfer equations are solved by deriving a Green's function. This yields the local radiative heat source needed to numerically solve the transient energy equation. An advantage of the two-flux method is that isotropic scattering is included without added complexity. The layer refractive indices are larger than one. This produces internal reflections at the boundaries and the internal interface; the reflections are assumed diffuse. Spectral results using the Green's function method are verified by comparing with numerical solutions using the exact radiative transfer equations. Transient temperature distributions are given to illustrate the effect of radiative heating on one side of a composite with external convective cooling. The protection of a material from incident radiation is illustrated by adding scattering to the layer adjacent to the radiative source.

Author

Radiative Transfer; Numerical Analysis; Boundaries; Incident Radiation; Heat Sources; Functional Analysis; Convective Heat Transfer

# 19970020072 Phillips Lab., Kirtland AFB, NM USA

# Structural Composite Penetration Model Development Final Report, 20 Mar. 1995 - 6 Feb. 1996

Chen, Jinn-Kuen, Phillips Lab., USA; Allahdadi, Firooz A., Phillips Lab., USA; Oct. 1996; 55p; In English Contract(s)/Grant(s): WAL-5-3063; AF Proj. 2402

Report No.(s): AD-A319784; PL-TR-96-1140; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

The Smoothed Particle Hydrodynamics (SPH) technique in conjunction with the macromechanics concept for fiber composites was developed to simulate impact penetration of composite structures, to describe the material behavior under high intensity loadings, a three dimensional anisotropic plasticity model, an equation of state, and a failure criterion for unidirectional composites were proposed. Furthermore, to maintain material frame indifference of the constitutive equations, the polar stress rate approach was employed in the stress and strain transformation under large rotation. The above physics were incorporated into SPH. Detailed penetration process and damage progression were simulated with graphite/epoxy composite laminates impacted by a steel projectile. The predicted impact response and damage patterns agree well qualitatively with the experimental results. This

study has demonstrated that SPH can be a robust and viable analytical tool for predicting response of fiber reinforced composite structures subjected to high velocity impact.

**DTIC** 

Composite Structures; Mathematical Models; Plastic Properties

19970020192 NASA Lewis Research Center, Cleveland, OH USA

Kinetics of Cyclic Oxidation and Cracking and Finite Element Analysis of MA956 and Sapphire/MA956 Composite System

Lee, Kang N., Cleveland State Univ., USA; Arya, Vinod K., Akron Univ., USA; Halford, Gary R., NASA Lewis Research Center, USA; Barrett, Charles A., NASA Lewis Research Center, USA; Metallurgical and Materials Transactions A; Oct. 1996; Volume 27A, pp. 3279-3291; In English

Report No.(s): NASA-TM-112757; NAS 1.15:112757; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Sapphire fiber-reinforced MA956 composites hold promise for significant weight savings and increased high-temperature structural capability, as compared to unreinforced MA956. As part of an overall assessment of the high-temperature characteristics of this material system, cyclic oxidation behavior was studied at 1093 C and 1204 C. Initially, both sets of coupons exhibited parabolic oxidation kinetics. Later, monolithic MA956 exhibited spallation and a linear weight loss, whereas the composite showed a linear weight gain without spallation. Weight loss of the monolithic MA956 resulted from the linking of a multiplicity of randomly oriented and closely spaced surface cracks that facilitated ready spallation. by contrast, cracking of the composite's oxide layer was nonintersecting and aligned nominally parallel with the orientation of the subsurface reinforcing fibers. Oxidative lifetime of monolithic MA956 was projected from the observed oxidation kinetics. Linear elastic, finite element continuum, and micromechanics analyses were performed on coupons of the monolithic and composite materials. Results of the analyses qualitatively agreed well with the observed oxide cracking and spallation behavior of both the MA956 and the Sapphire/MA956 composite coupons.

Author

Oxidation; Cracking (Fracturing); Finite Element Method; Fiber Composites; Crack Propagation; Kinetics; Matrix Materials

19970020226 Virginia Polytechnic Inst. and State Univ., Dept. of Civil Engineering, Blacksburg, VA USA

A Survey of Research on the Behavior and Mechanical Properties of Textile Composites

Suherman, Surjani, Virginia Polytechnic Inst. and State Univ., USA; Jul. 1996; 29p; In English

Contract(s)/Grant(s): DAAH04-95-I-0175

Report No.(s): AD-A316952; CE/VPI-ST-96/08; ARO-33421.3-EG; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Structures supported by a framework of inflated toroidal and cylindrical tubes would have relatively low weight and be easy to transport and erect. The tubes would be made of fabrics. Fabric composites have superior mechanical performance, such as high strength and low weight. In recent years, the development of textile structural composites has increased the need to investigate their behavior and effective properties. The properties can be controlled by changing the parameters, e.g., fiber orientation, fiber and matrix material properties, and fiber volume fraction. In this study, a survey of the research on the behavior and mechanical properties of textile composites of two common types, woven and braided, is presented. Various investigations, both analytical and experimental, are described. Elementary models, laminate theory models, and numerical (finite element) models are included in the review. Some programs that have been developed to calculate the mechanical properties of textile composites, such as TEX-CAD and FABCAD, are discussed. The failure behavior of textile composites is also surveyed.

**DTIC** 

Textiles; Composite Structures; Braided Composites; Woven Composites; Mathematical Models; Mechanical Properties

19970020296 SRI International Corp., Menlo Park, CA USA

Deformation and Failure of Metal-Matrix Composites Under Dynamic Loads Final Report, 1 Mar. 1992 - 31 Dec. 1995

Klopp, R. W., SRI International Corp., USA; Shockey, D. A., SRI International Corp., USA; Crocker, J. E., SRI International Corp., USA; Giovanola, J. H., SRI International Corp., USA; Dec. 22, 1996; 75p; In English

Contract(s)/Grant(s): F49620-92-C-0020; AF Proj. 2306

Report No.(s): AD-A320017; AFOSR-97-0022TR; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

SRI International conducted a three-year program of experiments, microstructural examinations, and analysis to determine the rate sensitivity of deformation and failure of metal-matrix composites (MMC) and to understand and model the role of interfaces and constituents on dynamic failure. Silicon-carbide fiber reinforced Timetal(R) 21S and Ti-15-3 matrices in three heat treatment conditions were studied. The work included dynamic fiber pushout experiments to measure dynamic interface strength,

notched three-point-bend experiments with acoustic emission sensors to determine the static fracture resistance, and notched one-point-bend experiments to determine dynamic fracture resistance. Microstructural examinations were performed on transverse and longitudinal cross sections. The nature of interface failure, fiber failure, and matrix failure was established. A key finding was that toughening from fiber bridging is not obtained under bending loads. In bending, fibers fail well in advance of the crack tip and are thereby prevented from bridg ing matrix cracks. A two-dimensional finite element model of the composite was developed in which fibers, matrix, and interfaces in the vicinity of the notch root were modeled explicitly. The model can be used in parameter studies to investigate changes in interface and constituent properties, and loading rate, and hence assist in designing MMCs having tailored combinations of strength, toughness, and, particularly, greater resistance to bend failure.

Metal Matrix Composites; Finite Element Method; Fiber Composites; Fracture Strength; Dynamic Loads; Deformation; Cracks; Failure; Crack Bridging; Titanium Alloys

19970020315 Illinois Univ., Dept. of Materials Science and Engineering, Urbana-Champaign, IL USA Transformation Weakening of Ceramic Composite Interfaces *Final Report*, 1 Apr. 1993 - 30 Mar. 1996

Kriven, Waltraud M., Illinois Univ., USA; Dec. 06, 1996; 71p; In English

Contract(s)/Grant(s): F49620-93-I-0227

Report No.(s): AD-A320605; AFOSR-TR-97-0064; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

Phase stability and transformations in some chosen ceramics was investigated and several new transformations in oxide systems were identified. To quantitatively understand the coupling of mechanical shear stress to nucleation, a constrictive double shear test was devised. It indicated that a minimum debonding shear strength of 95 MPa was needed to overcome the nucleation barrier for the proto (orthorhombic) to clino (monoclinic) transformation in enstatite (MgO.SiO2) and to give rise to 'transformational plasticity' in the polycrystalline ceramic. For comparison with transformation weakening, monazite (LaPO4) and zenotime (YPO4) fiber coatings were studied. Fiber pushout measurements indicated debonding shear strengths of 110-120 MPa were required for LaPO4 coatings, versus 95 MPa for YPO4, depending on coating thickness. A four layer, strong and damage tolerant oxide laminate was devised, based on YPO4, yttria stabilized zirconia (3 mol% Y2O3-ZrO2) and alumina (Al2O3), and having four point bend strengths of 392 MPa and work of fracture of approx. 10 KJ/sq m. Amorphous mullite (3Al2O.SiO2) and YAG (Y3Al5O12) fibers of tensile strengths 6.0 and 2.4 GPa respectively, were collaboratively fabricated and evaluated. Transformation weakening was demonstrated as a viable mechanism for interphase debonding in oxide systems. YPO4 demonstrated chemical compatibility in air with YAG (Y3Al5O12) and mullite (3Al2O3.SiO2) up to temperatures of 1600 C and 1500 C, respectively.

Ceramics; Composite Materials; Phase Transformations

19970020404 National Aerospace Lab., Tokyo, Japan

Friction, Wear and Electric Characteristics of Slip-ring Brush Materials for Space Applications, Part 2, Evaluation by Slip-ring simulation tests

Suzuki, Mineo, National Aerospace Lab., Japan; Watanabe, Mikio, National Aerospace Lab., Japan; Nishimura, Makoto, National Aerospace Lab., Japan; Nov. 1996; ISSN 0389-4010; 68p; In Japanese Report No.(s): NAL-TR-1315; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

Wear and electric characteristics of hot pressed Ag-MoS2-NbSe2 composites were evaluated in a vacuum environment in order to find the optimum brush material of a slip ring for space applications. The composite brush was rubbed against a coin silver ring or a silver ring, simulating a brush/ring contact of a slip-ring. First, the effect of the contacting load was evaluated under an electric current of 1 A and a sliding speed of 75 mm/s. The loads tested were 0.2 N, 0.6 N and 1 N. The increase in load resulted in lower electrical contact resistance and noise, and less wear. Better contact between the brush and the ring seemed to be responsible for the good performance. As the second step of the study, Ag-MoS2-NbSe2 composites with different contents of MoS2 and NbSe2 were evaluated under a load of 1 N and an electric current of from 1 A to 20 A. The best performance was obtained with an 85wt% Ag+12.5wt% MoS2+2.5wt% NbSe2 composite brush and a silver ring under both low-current (1A) and high-current (20A) conditions. Electrical contact resistance, electrical noise, and temperature and wear of the brush became extremely high as the electric current density increased. However, increasing the contact pressure of the brush was found to be very effective in lowering the electrical contact resistance and noise at high current density conditions. A high electric current density of 800 A/sq cm, with good electrical and wear resistance performance, was achieved at a contact pressure of 90 N/sq cm. Finally, the performance in nitrogen gas was examined because ground tests of a slip-ring for space use are carried out in nitrogen gas. The composite brush material developed in this study

is a promising candidate for a high power, small-sized, lightweight and long-lived slip-ring for future use in the space program to accommodate the increased power requirements.

Author (revised)

Friction; Wear Resistance; Electrical Resistance; Brushes; Molybdenum Disulfides; Composite Materials

# 25 INORGANIC AND PHYSICAL CHEMISTRY

Includes chemical analysis, e.g., chromatography; combustion theory; electrochemistry; and photochemistry. For related information see also 77 Thermodynamics and Statistical Physics.

19970019299 Georgia Univ., Athens, GA USA

Environmental Effects on High Energy Density Materials Final Report, 1 Sep. 1993 - 31 Aug. 1996

Schaefer, Henry F., III, Georgia Univ., USA; Oct. 10, 1996; 6p; In English

Contract(s)/Grant(s): F49620-93-1-0529; AF Proj. 2303

Report No.(s): AD-A317199; AFOSR-TR-96-0511; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The object of this research is to characterize, using ab initio quantum mechanical methods, the stabilizing or destabilizing effects of hydrogen and/or oxygen matrices on proposed high energy density molecular (HEDM) systems. In addition, the unimolecular fragmentation reactions of large HEDM species such as N20 will be studied via density functional methods. DTIC

Quantum Chemistry; Environment Effects; Chemical Reactions; Fragmentation; Molecules; Stabilization; Hydrogen; Oxygen

#### 19970019306 Argonne National Lab., IL USA

#### Chemical decomposition by normalization of millimeter-wave spectra

Gopalan, K., Purdue Univ., USA; Gopalsami, N., Argonne National Lab., USA; [1996]; 7p; In English; IEEE Instrumentation and Measurement Technology Conference, 4 - 6 Jun. 1996, Brussels, Belgium

Contract(s)/Grant(s): W-31109-ENG-38

Report No.(s): ANL/ET/CP-91028; CONF-9606271-1; DE96-015070; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The sharp, distinct absorption spectra of chemicals at low pressures in the mm wave range become broadened at high pressures, so that detecting and quantifying different chemicals at high pressures become difficult. This paper proposes a method of decomposition based on the low pressure spectra. Normalized low pressure spectral amplitudes are used as features to train a neural network. The network is tested using the peak spectra obtained for an unknown plume of chemicals at high pressure. Initial tests conducted on simulated and experimental spectra of selected chemicals show that the decomposition results of the proposed method are dependent on the dominance of the chemicals in the mixture - a characteristic common to conventional methods of decomposition.

DOE

Absorption Spectra; Decomposition; Normalizing (Heat Treatment); Organic Compounds; Absorption Spectroscopy; Detection; Millimeter Waves: Plumes

19970019313 Lawrence Livermore National Lab., Dept. of Chemistry and Materials Science, Livermore, CA USA Capacitive Deionization of NH4ClO4 Solutions with Carbon Aerogel Electrodes *Final Report, Oct. 1994 - Jun. 1995* 

McSweeney, Kevin T., Lawrence Livermore National Lab., USA; Morris, Dave, Lawrence Livermore National Lab., USA; Rettle, Bob, Lawrence Livermore National Lab., USA; Kelley, Stephen E., Lawrence Livermore National Lab., USA; Aug. 15, 1996; 58p; In English

Contract(s)/Grant(s): W-7405-eng-48

Report No.(s): AD-A318501; AL/EQ-TR-1995-0038; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

A process for the capacitive deionization of water with a stack of carbon aerogel electrodes has been developed by Lawrence Livermore National Laboratory. Unlike ion exchange, one of the more conventional deionization processes, no chemicals are required for regeneration of the system. Electricity is used instead. Water with various anions and cations is pumped through the electrochemical cell. After polarization, ions are electrostatically removed from the water and held in the electric double layers

formed at the surfaces of electrodes. The water leaving the cell is purified, as desired. The effects of cell voltage and cycling on the electrosorption capacities for NH4ClO4 and NaCl have been investigated and are reported here.

DTIC

Aerogels; Deionization; Carbon; Ammonium Perchlorates; Capacitance; Electrolytes

19970019320 New Mexico Univ., Center for Micro-Engineered Materials, Albuquerque, NM USA

Hydrolysis and Condensation of Tin(IV) Alkoxide Compounds: The Control of Structural Evolution Final Report, 15 Apr. 1993 - 14 Apr. 1996

Hampden-Smith, M. J., New Mexico Univ., USA; Jun. 1996; 7p; In English

Contract(s)/Grant(s): F49620-93-1-0197; AF Proj. 2303

Report No.(s): AD-A318484; AFOSR-96-0552TR; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

We have studied ester elimination in a number of model systems to determine the criteria which promote or inhibit such reactions. The model systems generally involve metal centers which possess NMR active nuclei such as 29Si, 119, 117Sn and 207Pb. In these systems, we have conducted a number of 170 labeling experiments which reveal that ester elimination is probably an associative process that requires electropositive metal alkoxide centers, accessible coordination sites at the metal centers, dangling carboxylate ligands and which is promoted by noncoordinating solvents and inhibited by coordinating solvents. In a heterobimetallic systems, the reaction between Sn(O-t-Bu)4 and Pb(OAc)4 results in formation of a metal oxo cluster in the presence of toluene. These metal oxo clusters retain their structure in solution as determined by multinuclear NMR, spectroscopy for PbSn2O(O-t-Bu)4(OAc)4. As a result of this understanding gained from these model reactions, we are now in a position to investigate the formation of metal oxide materials using these clusters.

DTIC

Alkoxides; Esters; Hydrolysis; Tin Compounds; Condensation; Metal Clusters; Organometallic Compounds

19970019323 State Univ. of New York, Dept. of Chemistry, Buffalo, NY USA

Main Group Compounds as Amphoteric Ligands to Transition Metals. Synthesis and Molecular Structure of Cr(CO)5 PPh2CH2Ga (CH2CMe3)2, NMe3

Beachley, O. T., Jr., State Univ. of New York, USA; Banks, Michael A., State Univ. of New York, USA; Kopasz, John P., State Univ. of New York, USA; Rogers, Robin D., State Univ. of New York, USA; Jul. 10, 1996; 26p; In English Contract(s)/Grant(s): N00014-96-I-0483

Report No.(s): AD-A317459; TR-45; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The reactivities of the group 13 compounds, R2MCH2PPh2 and R2MPPh2, as amphoteric ligands to transition metals have been investigated. The ligands R2MCH2PPh2 (R = CH2CMe3, CH2SiMe3; M = Ga, In) reacted readily with Cr(CO)5NMe3 in benzene solution to form Cr(CO)5PPh2CH2MR2-NMe3 whereas for ligands of the type R2MPPh2 (R = CH2CMe3, CH2SiMe3; M = Al, Ga, In), only the two aluminum compounds and (Me3CCH2)2GaPPh2 formed isolable products of the type Cr(CO)5PPh2MR2-NMe3. However, the gallium and indium ligands with trimethylsilylmethyl substituents (Me3SiCH2)2MPPh2 reacted with NEt4MT(CO)5Cl (MT = Cr, Mo, W) to form products of the type NEt4MT(CO)5PPh2MR2Cl. All new compounds were characterized by their physical properties, C and H analyses, and 1H and 31P NMR and IR spectral properties. The identity of NEt4Cr(CO)5PPh2In(CH2SiMe3)2Cl was further confirmed by the subsequent identification of products from reactions with anhydrous HCl and with MeI. In addition, Cr(CO)5PPh2CH2Ga(CH2CMe3)2.NMe3 was characterized by an X-ray structural study.

DTIC

Transition Metals; Molecular Structure; Chromium Compounds

19970019328 Army Cold Regions Research and Engineering Lab., Hanover, NH USA

**Sampling Trace-Level Organics with Polymeric Tubings** 

Parker, Louise V., Army Cold Regions Research and Engineering Lab., USA; Ranney, Thomas A., Science and Technology Corp., USA; Oct. 1996; 37p; In English

Report No.(s): AD-A319954; CRREL-SR-96-3; SFIM-AEC-ET-CR-95072; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

There is concern whether tubings used to sample groundwater can affect contaminant concentrations. Tubings might sorb contaminants, thereby giving falsely low values, or they might leach contaminants, thereby giving falsely high values. There also is concern that a tubing used previously in a well with high concentrations of contaminants might subsequently desorb contaminants into samples taken from other wells if decontamination is insufficient. Our review of the literature indicated that these concerns are valid, although a comprehensive study of this subject does not exist. In our laboratory study, we looked for sorption of a suite of organic solutes by 20 polymeric tubings under static conditions. Seven of these tubings were flexible and the others were

rigid. We found that among the rigid tubings tested, the three fluoropolymers (fluorinated ethylene propylene (FEP), FEP-lined polyethylene, and polyvinylidene fluoride (PVDF) were the least sorptive tubings. However, even these tubings readily sorbed some of the analytes. Among the flexible tubings tested, a fluoroelastomer tubing and a tubing made of a copolymer of vinylidene fluoride and hexafluoropropylene (PVDF-HFP) were the least sorptive. We also found that several of the 20 tubings appeared to leach constituents into the test solution. We were unable to detect any evidence that constituents leached from the polyethylene tubings, the rigid fluoropolymer tubings, and one of the plasticized polypropylene tubings. Currently, we are conducting studies to see whether the effects we observed in this study increase, decrease, or remain the same under dynamic conditions. DTIC

Ground Water; Pipes (Tubes); Contaminants; Sorption; Fluoropolymers; Copolymers

19970019332 Edgewood Research Development and Engineering Center, Aberdeen Proving Ground, MD USA Interaction of VX-, G-, and HD-Simulants with Self-Decontaminating Sorbents: A Solid-State MAS NMR Study Final Report, Dec. 1995 - Jun. 1996

Wagner, George W., Geo-Centers, Inc., USA; Bartram, Phillip W., Edgewood Research Development and Engineering Center, USA; Nov. 1996; 25p; In English

Contract(s)/Grant(s): DAAM01-94-C-0047

Report No.(s): AD-A318809; ERDEC-TR-375; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

P and C MAS NMR were used to follow the reactions of simulants for VX (DEPPT), HD (CEPS\*), and G agents (DFP) on commercial aluminas, XE-555 and a polydivinylbenzene impregnated with polyethylenimine, polyethylene gylcol, and sodium hydroxide (DVB-PNP). The several aluminas examined showed comparable DEPPT reactivity. The alumina hydration state affected DEPPT and CEPS\* reactivity. The DVB-PNP prepared with MeOH, rather than H2O, was much more reactive towards DEPPT and DFP. Reactions of DEPPT and DFP with DVB-PNP (MeOH) were too fast to measure (t(sub 1/2) less than 5 min). For DFP applied to XE-555, competing reaction and micropore-adsorption processes were observed.

Reactivity; Nuclear Magnetic Resonance; Sorbents; Humidity; Aluminum Oxides; Polyethylenes

19970019394 Centro de Investigaciones Energeticas, Metrologia de Radiaciones Ionizantes, Madrid (Spain). Madrid, Spain Electrodeposition of Radium *Electrodeposicion del Radio* 

Crespo, M. T., Centro de Investigaciones Energeticas, Spain; Jimenez, A. S., Centro de Investigaciones Energeticas, Spain; 1996; 15p; In Spanish

Report No.(s): CIEMAT-800; DE97-703827; INIS-ES-9600172; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche A study of different electrodeposition methods of radium for its measurement by alpha-spectrometry is presented. The recommended procedure uses an aqueous solution of ammonium oxalate and nitric acid in the presence of microgram amounts of platinum as electrolyte.

DOE

Electrodeposition; Ammonium Compounds; Nitric Acid; Oxalates; Platinum; Radium

19970019400 Lawrence Livermore National Lab., Livermore, CA USA

#### **Liquid filtration simulation**

Corey, I., Lawrence Livermore National Lab., USA; Bergman, W., Lawrence Livermore National Lab., USA; Jun. 1996; 21p; In English

Contract(s)/Grant(s): W-7405-ENG-48

Report No.(s): UCRL-ID-124336; DE96-050513; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

We have a developed a computer code that simulates 3-D filtration of suspended particles in fluids in realistic filter structures. This code, being the most advanced filtration simulation package developed to date, provides LLNL and DOE with new capabilities to address problems in cleaning liquid wastes, medical fluid cleaning, and recycling liquids. The code is an integrated system of commercially available and LLNL-developed software; the most critical are the computational fluid dynamics (CFD) solver and the particle transport program. For the CFD solver, we used a commercial package based on Navier-Stokes equations and a LLNL-developed package based on Boltzman-lattice gas equations. For the particle transport program, we developed a cod based on the 3-D Langevin equation of motion and the DLVO theory of electrical interactions. A number of additional supporting packages were purchased or developed to integrate the simulation tasks and to provide visualization output.

Computer Programs; Computerized Simulation; Filtration; Liquid Wastes; Equations of Motion; Recycling

19970019410 Forschungszentrum Karlsruhe G.m.b.H., Inst. fuer Radiochemie, Karlsruhe, Germany

Practical surface analysis. Contributions to a workshop at the Karlsruhe Research Centre on November 9-11, 1994 Praktische Oberflaechenanalytik. Beitraege zu einem Workshop im Forschungszentrum Karlsruhe vom 9.-11. November 1994 Goschnick, J., Editor, Forschungszentrum Karlsruhe G.m.b.H., Germany; Schuricht, J., Editor, Forschungszentrum Karlsruhe G.m.b.H., Germany; Dec. 1995; ISSN 0947-8620; 206p; In German; Practical Surface Analysis Workshop, 9 - 11 Nov. 1994, Karlsruhe, Germany

Report No.(s): FZKA-5691; CONF-9411317-; DE96-770575; No Copyright; Avail: CASI; A10, Hardcopy; A03, microfiche; US Sales Only; US Sales Only

This volume contains 22 lectures which were given at the Workshop 'Practical Surface Analysis' at the College for Technology and the Environment of the Karlsruhe Research Centre. The subjects were: SIMS for detecting the depth distribution; measuring the thickness of layers with SNMS; surface and depth profile analysis of ceramic powders; analysis of aerosol particles resolved according to depth with SNMS and SIMS; individual particle analysis of atmospheric microparticles; determining the origin of the emission of fine dust; the analysis of smoke particles in dense smoke from fires; fast soil analysis of historic waste dumps; surface analysis of semiconductor structures (SIMS); depth profile measurements on glass after anodic bonding with copper; principles of photo-electron spectroscopy and AES; the use of the surface analysis processes AES, XPS and SIMS in material testing; analysis of ionic glasses for electro-chemical microsensors; analysis of CVD layers for gas sensors; characterisation of wool with surface modified by corona discharge; corrosion on metals; atmospheric damage to metal surfaces and passivation of steel in aggressive media; electron microscope processes in material testing; quantitative X-ray micro-analysis of PVC layers for microsystem technique; photo-thermal analysis of metal surfaces after atmospheric corrosion; the application of the scanning microscope to biological material.

DOE

Conferences; Aerosols; Metal Surfaces; Microanalysis; Microparticles; Gas Detectors; Powder (Particles); X Ray Spectroscopy

19970019495 Joint Inst. for Nuclear Research, Dubna, USSR

The use of physical methods for elemental analysis of ecological samples Ispol'zovanie fizicheskikh metodov dlya ehlementnogo analiza ehkologicheskikh obraztsov

Kudryashov, V. I., Leningrad State Univ., USSR; Zhuravleva, E. L., Joint Inst. for Nuclear Research, USSR; Maslov, O. D., Joint Inst. for Nuclear Research, USSR; 1996; 11p; In Russian

Report No.(s): JINR-18-96-161; DE97-605643; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

The possibility of the application of difference X-ray and instrumental activation methods elemental analysis of rock ice, snow, water, soil and other natural samples was investigated. The content of some elements in ice samples from the glaciers of the Pamirs-Alaj mountain system for period 1973-1984 years has been determined. The recommendations for the choice of analysis methods with the aim of the environmental control have been given.

DOE

Ecology; Neutron Activation Analysis; X Rays; Fluorescence

19970019541 Drexel Univ., Dept. of Mechanical Engineering, Philadelphia, PA USA

Development of a Reduced Chemical Kinetic Model for Prediction of Preignition Reactivity and Autoignition of Primary Reference Fuels

Li, Houliang, Drexel Univ., USA; Miller, David L., Drexel Univ., USA; Cernansky, Nicholas P., Drexel Univ., USA; Jul. 23, 1996; 19p; In English

Contract(s)/Grant(s): DAAH04-93-G-0042

Report No.(s): AD-A317165; ARO-30782-8-EG; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

A reduced chemical kinetic model has been developed for the prediction of major oxidation behavior of Primary Reference Fuels (PRF's) in a motored engine, including ignition delay preignition heat release, fuel consumption, CO formation and production of other species classes. This model consists of 29 reactions with 20 active species and was tuned to be applicable for the neat PRF's, 87 PRF and 63 PRF, and at various engine conditions. At the motored engine condition where detailed species data were generated, the model reproduces the ignition delay and the preignition heat release quite well (to within 15%). Fuel consumption and CO formation predictions differed from experiments by at most 25% for all of the four fuels. Predictions for other species classes generally agreed with experiments. As inlet temperature was varied, the experimentally observed Negative Temperature

Coefficient (NTC) behavior of iso-octane and 87 PRF was reproduced by the model. In addition, the lower reactivity of 87 PRF at a lower compression ratio was also predicted, indicating that the model can account for the effects of pressure or charge density. DTIC

Chemical Reactions; Dynamic Models; Reaction Kinetics

19970019548 Arkansas Univ., Fayetteville, AR USA

## Photothermal Investigations of GaAs-Based Materials and Quantum-Well Structures Final Report

Gupta, R., Arkansas Univ., USA; Vyas, R., Arkansas Univ., USA; Ang, S., Arkansas Univ., USA; Brown, W. D., Arkansas Univ., USA; Aug. 02, 1996; 22p; In English

Contract(s)/Grant(s): F49620-92-J-0381; AF Proj. 2305

Report No.(s): AD-A316435; AFOSR-TR-96-0499; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Photothermal deflection spectroscopy has been applied to GaAs samples with the ultimate goal of measuring the optoelectronic and thermal transport properties of GaAs based multiple quantum wells by this technique. Theoretical models have been developed as well as experimental investigations have been carried out. Both pulsed as well as cw (modulated) excitations have been considered.

**DTIC** 

Gallium Arsenides; Quantum Wells; Continuous Radiation; Thermodynamic Properties; Transport Properties

19970019552 Florida Univ., Dept. of Chemistry, Gainesville, FL USA

Transition Metal Complex Superconductors by Electrocrystallization: Nonmetallic and Bimetallic Chalcogen-Rich, Extensively Conjugated and Planar Complexes for Highly Electrically Conducting Materials *Final Report*, 1 Jun. 1993 - 31 May 1996

Reynolds, John R., Florida Univ., USA; Sep. 23, 1996; 19p; In English

Contract(s)/Grant(s): F49620-93-I-0322; AF Proj. 3484

Report No.(s): AD-A317220; AFOSR-TR-96-0517; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

A series of monometallic and bimetallic transition metal complexes have been synthesized for incorporation into highly conductive and potentially superconductive materials. Studies of Ni(dmit)2C(+)(x), as a function of cation C(+) type, have allowed elucidation of the effect of structure on electronic properties. A new class of bimetallic TetraThioOxalate (TTO) bridged compounds were discovered that form new synthetic conductors. For example, the reaction of (Bu4N)2(tto(Ni(dmit)2) with (TTF)3(BF4)2 led to a material with a conductivity of 0.4 S/cm. A full study of seven new bimetallic, and one new tetrametallic, complex has been carried out with single crystal X-ray structures determined.

Transition Metals; Bimetals; Cations

19970019556 Centro de Isotopos, Havana, Cuba

Radioiodination of the protein complex of the VA-MENGOC-BC vaccine Yodacion del complejo proteico VA-MENGOC-BC

Caso, R., Centro de Isotopos, Cuba; Lastre, M., Centro de Investigacion Produccion de Vacunas y Sueros, Cuba; Alvarez, L., Instituto Superior de Ciencia y Tecnologia Nuclear, Cuba; 1996; 9p; In Spanish

Report No.(s): CIEN-R-43-96; DE97-603940; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche; US Sales Only; US Sales Only

In this work was made the labelling of the protein complex of the vaccine VA-MEMGOC-BC with I-125 in order to study its immunological responses. These proteins were in both forms: dissolved and conjugated with polisacarids of the C-group. There were used three methods of iodination: chloramine-T iodogen and lactoperoxidase. Was found out that dissolved proteins can be iodinated using these methods with 0,1 mCi of I-125, and the obtained specific activities were similar.

DOE

D ( ' 17 ' 1

Proteins; Vaccines; Immunology

19970019573 Case Western Reserve Univ., Dept. of Natural Sciences and Engineering, Cleveland, OH USA Processing and Properties of Tough Silicides

Lewandowski, John J., Case Western Reserve Univ., USA; Aikin, Robert M., Jr., Case Western Reserve Univ., USA; May 1996; 62p; In English

Contract(s)/Grant(s): F49620-93-I-0092

Report No.(s): AD-A320473; AFOSR-TR-97-0043; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

The processing and properties of tough silicides have been investigated. Vacuum hot pressing was utilized to produce Nb5Si3/Nb laminates, while the fracture toughness of the laminates was evaluated with the use of a deformation stage situated inside of a SEM. The interface strength in such laminates was systematically varied as was the thickness of the Nb layer in order to determine the effects of such changes on the fracture behavior and toughness of such laminates. The effects of changes in test temperature on the above were also determined. Complementary experiments were conducted on in-situ composites where R-curve behavior was obtained. In addition, the effects of changes in grain size, test temperature, and alloy content, on the cleavage fracture stress and the fracture toughness were determined. The results of these experiments were used to rationalize the fracture behavior of the laminates and in-situ composites.

DTIC

Silicides; Hot Pressing; Niobium Compounds; Fracture Strength; Laminates

19970019614 Materials Research Society, Pittsburgh, PA USA

Gallium Nitride and Related Materials, Volume 395 Final Report, 25 Sep. 1995 - 28 Sep. 1996

Pachavis, Robert H., Materials Research Society, USA; Ponce, F. A., Editor, Xerox Palo Alto Research Center, USA; Dupuis, R. D., Editor, Texas Univ., USA; Nakamura, S., Editor, Nichia Chemical Industries Ltd., Japan; Edmond, J. A., Editor, Cree Research, Inc., USA; Sep. 1996; 949p; In English, 27 Nov. - 1 Dec. 1995, Boston, MA, USA

Contract(s)/Grant(s): DAAH04-95-I-0646

Report No.(s): AD-A317312; ARO-35016.2-MS-CF-Vol-395; No Copyright; Avail: Issuing Activity (Defense Technical Information Center (DTIC)), microfiche

The current excitement in the scientific community about the III-V nitrides was reflected in this First International Symposium on Gallium Nitride and Related Materials (ISGN-1). The symposium consisted of nine half-day oral sessions (25 invited and 54 contributed talks) and four poster Sessions (113 presentations). The attendance was very high for all sessions, with an estimated peak of over 550 attendees at one of the sessions. The symposium reflected the large amount of work that has taken place since the field exploded about two years ago with the announcement of commercial blue light emitting devices. The invited talk program was designed to give a thorough review of the state of the art in the field. The large number of contributions, in the form of talks and poster presentations, showed much progress in understanding III-V nitrides, and in the production of optoelectronic devices based on these materials. These proceedings represent the current state of understanding in the field, reflecting about 75% of the work presented at the symposium.

**DTIC** 

Gallium Nitrides; Optoelectronic Devices; Conferences

19970019626 Army Research Lab., Aberdeen Proving Ground, MD USA

Investigation of Possible Decomposition of Alternative Fire-Extinguishing Agents Discharged Through a Vehicle Personnel Heater *Final Report, Jun. 1995 - Jan. 1996* 

McNesby, Kevin L., Army Research Lab., USA; Modiano, Steven H., Army Research Lab., USA; Marsh, Paul, Army Test and Evaluation Command, USA; Bolt, William, Army Test and Evaluation Command, USA; Herud, Craig, Army Test and Evaluation Command, USA; Oct. 1996; 49p; In English

Contract(s)/Grant(s): DA Proj. 1L1-61102-AH-43

Report No.(s): AD-A316811; ARL-TR-1207; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Fourier transform infrared (FT-IR) spectroscopy was used to monitor the possible thermal decomposition of alternative fire-extinguishing agents discharged through a vehicle personnel heater. The agent was introduced into the heater air induction pen and flowed across the heat exchanger manifold. Gas samples were removed from the hot air output duct extension of the heater via stainless steel tubing and flowed through a 10m path-length multipass optical gas cell placed in the sample beam of an PT-IR spectrometer. Five fire-extinguishing agents, CF3Br (trade name, Halon 1301), C3F7H (FM-200), C3F6H2 (FE-36), C2F5H (FE-25), and CF3H (FE-13), were tested for two manifold temperatures of 380 and 480-510 deg C. No agent decomposition or combustion gas products could be detected for any of the agents tested under these temperature conditions. The agent decomposition products of interest were HF, HBr, CO, CF3H, C2H2, CH4, C2H4, and CF2O.

Fire Extinguishers; Combustion Products; High Temperature Air; Heat Exchangers

19970019700 Army Research Lab., Aberdeen Proving Ground, MD USA

Temperature Dependent Microwave Absorption in Selected Nitrates and Nitrites *Final Report, Jan. 1993 - Sep. 1995* Cornelison, Steven G., Army Research Lab., USA; Gauss, Arthur, Jr., Army Research Lab., USA; Krane, J., Nebraska Univ., USA; Hardy, J. R., Nebraska Univ., USA; Aug. 1996; 30p; In English

Contract(s)/Grant(s): DA Proj, 1L1-61102-AH-43

Report No.(s): AD-A317746; ARL-TR-1179; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Molecular dynamics studies performed at the University of Nebraska have predicted that microwave activity should be present in some ionic molecular crystals and that significant dielectric losses may occur at or near order/disorder transition temperatures. Temperature-dependent centimeter reflection studies at frequencies from 2 to 20 GHz were performed at the U.S. Army Research Laboratory (ARL) on powdered samples of potassium nitrate, potassium nitrite, sodium nitrate, and sodium nitrite. The measurements, which show significant dielectric losses in some cases, are compared to calculations based on a Debye relaxation model. Losses observed in the salts containing nitrite ions are expected to be due to the presence of permanent dipole moments that are excited to hopping modes as the temperature is raised. Losses observed in potassium nitrate are expected to be due to the development of 'induced' dipole moments as the material nears its order/disorder transition temperature of 128 deg C. DTIC

Microwave Absorption; Molecular Dynamics; Transition Temperature

19970019728 Georgia Univ., Dept. of Chemistry, Athens, GA USA

Electrochemical Formation of CdSe Monolayers on the Low Index Planes of Au, 1 Jun. 1995 - 15 Oct. 1996

Lister, T. E., Georgia Univ., USA; Colletti, L. P., Georgia Univ., USA; Stickney, J. L., Georgia Univ., USA; Oct. 15, 1996; 36p; In English

Contract(s)/Grant(s): N00014-19-J-1919

Report No.(s): AD-A317313; GU-TR-26; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The electrochemical analog of atomic layer epitaxy (ALE) is being studied. ALE is a method for growing thin films of materials using a cycle of surface limited reactions. The surface limited reactions control the deposition by limited the growth to an atomic layer at a time. In electrochemistry, a surface limited deposition is generally referred to as under-potential deposition (UPD), and UPD is used to form the atomic layers in electrochemical ALE (ECALE). The work presented here is an atomic level study of the deposition of the first few monolayers of CdSe via ECALE: by the alternated UPD of atomic layers of Se and Cd on the low index planes of Au. UPD of Se resulted in the formation of ordered structures on each of the low index planes of Au, as observed by low energy electron diffraction (LEED) and scanning microscopy (STM). The subsequent UPD of Cd resulted in CdSe deposits which exhibited 1:1 stiochiometry, as determined by coulometry and Auger electron spectroscopy (AES). The following LEED patterns were observed for the CdSe monolayers: Au(111) (square root of 7 times square root of 7)Rl9.1deg2, Au(111)(3 X 3), Au(110)(2 X 3), and the Au(100)(square root of 2 times square of 2)R45 deg. Similar LEED patterns were observed on each surface for deposits formed using up to three ECALE cycles.

Cadmium Selenides; Atomic Layer Epitaxy; Auger Spectroscopy; Electrochemistry; Surface Reactions; Thin Films; Electrode-position; Electron Spectroscopy

19970019757 California Inst. of Tech., Pasadena, CA USA

Living Catalysts for Cyclohexadiene Polymerization Final Report, 1 Jun. 1995 - 31 May 1996

Grubbs, Robert H., California Inst. of Tech., USA; Jul. 31, 1996; 4p; In English

Contract(s)/Grant(s): F49620-92-J-0483

Report No.(s): AD-A317606; AFOSR-TR-96-0535; No Copyright; Avail: CASI; A01, Hardcopy; A01, microfiche

Rhenium Oxovinylalkylidene Complex (ROMP) polymerization has become an important method for the preparation of polyphenylenevinylenes and polynaphthylenevinylene. The new route allows the band gap and processing properties of the polymers to be varied by the use of side chains and functional groups. These materials are being used to fabricate electoluminescent devices with tunable colors. New techniques have been developed for the synthesis of the starting barrelenes and benzobarrelenes. The synthesis starts from the ICI diol system that was used in the preparation of polyparaphenylene. A key to these developments is the availability of well defined catalysts. Considerable effort has been devoted to the design and synthesis of new complexes that will catalyze the ROMP polymerization reaction and to develop new procedures which will control the molecular weight and livingness of those systems know. The students involved in this work have gained experience in polymer synthesis, catalyst development and the fabrication of devices.

**DTIC** 

Cyclic Compounds; Vinyl Radical

19970019876 Centro de Estudios Aplicados al Desarrollo Nuclear, La Habana, Cuba

Determination of selenium in Ni + Co concentrates applying epithermal neutron activation analysis Determinacion de selenio en muestras de concentrados de niquel mas cobalto empleando el analisis por activacion con neutrones epitermicos

Capote Rodriguez, G., Centro de Estudios Aplicados al Desarrollo Nuclear, Cuba; Perez Sayaz, G., Centro de Estudios Aplicados al Desarrollo Nuclear, Cuba; Hernandez Rivero, A., Centro de Isotopos, Cuba; Moreno Bermudez, J., Centro de Isotopos, Cuba; Ribeiro Guevara, S., Comision Nacional de Energia Atomica, Argentina; Arribere, M.A., Comision Nacional de Energia Atomica, Argentina; Molina Insfran, J., Universidad Nacional de Asuncion, Paraguay; 1996; 11p; In Spanish

Report No.(s): CIEN-R-41-96; DE97-601004; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche; US Sales Only; US Sales Only

Concentration of Se in Ni + Co concentrates obtained in nickel industry has to be determined as that is a quality control requirement for its commercialization. At present, analysis of Se, specially at a minor and trace levels is relatively complicated and destructive procedures are frequently required. In this work determination of Se by epithermal neutron activation analysis (ENAA) in 17 samples of nickel industry was investigated. Application of ENAA allowed nondestructive determination of Se concentration down to ppm level in spite of presence of high Co, Fe, Ni, and Cr contents in the samples.

Quality Control; Commercialization; Selenium; Nickel

19970019885 Prins Maurits Lab. TNO, Rijswijk, Netherlands

Experimental Field Study of Evaporation of Deposited Droplets of Chemical Agents from Various Substrates *Final Report* Oeseburg, F., Prins Maurits Lab. TNO, Netherlands; Him, A. R., Prins Maurits Lab. TNO, Netherlands; Aug. 1996; 290p; In English; Original contains color plates

Contract(s)/Grant(s): A95/KL/455

Report No.(s): AD-A316373; PML-1995-A87; TD95-1565; No Copyright; Avail: CASI; A13, Hardcopy; A03, microfiche

Existing models for surface evaporation of droplets of chemical agents are unreliable, mainly because the size of the experimental data-sets, on which these models are based, often are too small. Furthermore, the accuracy of the data is limited because downwind vapour sampling was generally used as measuring method to determine the evaporated mass and it is well known that this method is supposed to be unreliable. In order to obtain a reliable data set, TNO-PML started an experimental programme including field (only simulants) and wind-tunnel (simulant as well as live agents) experiments. This report contains the result of the field trials. During these experiments, droplets of simulant (total mass on substrate approx. 200 to 300 mg) were placed onto a circular surface of the substrate (diameter about 11 cm) and the mass of the contaminated substrates was recorded as a function of time, using an ordinary laboratory balance. Glass, artificial grass and sand were used as substrate material. Neat agent (DiEthyl-Malonate (DEM) and MethylSalicylate (MS)) and thickened agent (DEM) were applied. The volumes of the droplets amounted to 1 micro 1 (neat agent on glass and artificial grass), 5 micro 1 (neat on sand) and 14 micro 1 (thickened on all substrates). In order to correct for possible mass changes of the substrate material itself, mass-time profiles of clean substrates were recorded simultaneously (reference balance). In addition, the mass residue with the agent at the endpoint of the experiment was measured using extraction in combination with GC. During the experiments a number of relevant physical quantities (windspeeds at 0.01, 0.025, 0.05, 0.1, 0.5, 2.5 and 10 m; substrate surface temperature; air temperature; relative humidity) were measured as well (sample frequency 0.1 Hz). In total about 40 experiments were carried out during the months May - October. DTIC

Surface Temperature; Frequencies; Humidity; Residues

19970019902 Kyoto Univ., Research Reactor Inst., Kumatori, Japan

#### Proceedings of Workshop on Boron Chemistry and Boron Neutron Capture Therapy

Kitaoka, Yoshinori, Editor, Kyoto Univ., Japan; Oct. 1995; 69p; In Japanese; In English; Fundamental Knowledge and Application of Neutron Activation Analysis by a Reactor, 15-16 Feb. 1994, Kumatori, Japan

Report No.(s): KURRI-TR-413; CONF-9402147; DE97-711190; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche This issue is the collection of the paper presented at the Workshop on Boron Chemistry and Boron Neutron Capture Therapy. Eight of the presented papers are indexed individually. DOE

Conferences; Boron 10; Capture Effect; Neutrons; Therapy

19970019988 NASA Goddard Space Flight Center, Greenbelt, MD USA

A Comparison of Atomic Oxygen Degradation in Low Earth Orbit and in a Plasma Etcher

Townsend, Jacqueline A., NASA Goddard Space Flight Center, USA; Park, Gloria, NASA Goddard Space Flight Center, USA;

Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 295-304; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

In low Earth orbit (LEO) significant degradation of certain materials occurs from exposure to atomic oxygen (AO). Orbital opportunities to study this degradation for specific materials are limited and expensive. While plasma etchers are commonly used in ground-based studies because of their low cost and convenience, the environment produced in an etcher chamber differs greatly from the LEO environment. Because of the differences in environment, the validity of using etcher data has remained an open question. In this paper, degradation data for 22 materials from the orbital experiment Evaluation of Oxygen Interaction with Materials (EOIM-3) are compared with data from EOIM-3 control specimens exposed in a typical plasma etcher. This comparison indicates that, when carefully considered, plasma etcher results can produce order-of-magnitude estimates of orbital degradation. This allows the etcher to be used to screen unacceptable materials from further, more expensive tests.

Earth Orbital Environments; Low Earth Orbits; Oxygen Atoms; Degradation; Spacecraft Shielding; Spacecraft Construction Materials

#### 19970019990 Naval Surface Warfare Center, Dahlgren, VA USA

# The Oxidation of Refractory Elements and Compounds in an Atomic Oxygen Environment

Opeka, Mark M., Naval Surface Warfare Center, USA; Rapp, Robert A., Ohio State Univ., USA; Wuttig, Manfred, Maryland Univ., USA; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 315-331; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A03, Hardcopy; A04, microfiche

An analytical methodology was developed to predict the behavior of elements and compounds in atomic oxygen (AO) environments. Thermodynamic condensed and vapor phase equilibria were calculated in order to compare the responses to AO and to O2 of a broad range of materials. The materials included Cu, Ag, Au, Pd, Pt, Rh, Ir, Ru, Os, Re, Cr, Mo, W, Al, Si, Be, C, B, Ti, TiC, TiN, and TiB2. An experimental apparatus was constructed in order to evaluate the AO-oxidation behavior of selected materials. AO was produced by an N2 dissociation/NO titration technique to yield thermal AO. AO response experiments at a P(sub o) (O-atom pressure) of 10(exp -5) atm (1 atm = 101.3 kPa) and at temperatures of up to 675 K were conducted with Au, Ru, Ti, TiC, and TiB2. The condensed phase equilibria calculations indicated that four metals -- Ag, Au, Ru, and Cr -- form different condensed oxides in AO (P(sub o) = 7(exp -7) atm) than in air at 300 K, suggesting that oxidation rates will differ. The vapor phase equilibria calculations indicated that seven metals -- Os, Ru, Ir, Pt, Re, Cr, and Mo -- may exhibit significant vaporization rates in AO (Po = 10(exp -7) atm) at low temperatures (300 K to 1000 K, depending on the metal). Using a vaporization model which includes O-atom supply limitations, the predicted vaporization rates for Os, Ir, Re, and Cr correlate well with published measurements. Experimentally, Au and Ru did not oxidize according to AO-based thermodynamics. The results suggest that high O-to-O2 recombination coefficients for these metals significantly decreased P(sub o) at the surface. TiC exhibited logarithmic kinetics in AO at 675 K, in qualitative agreement with published O2 oxidation results for Ti and TiC. The thermodynamic prediction methodology developed in this research provides the first systematic framework to understand and predict the response of elements and compounds to AO. It has been found to be a powerful tool for understanding AO-oxidation behavior and for predicting the temperature dependence of vaporization rates. Author

Oxygen Atoms; Oxidation; Gas Dissociation; Thermodynamics; Temperature Dependence; Refractories

# 19970019993 Jet Propulsion Lab., California Inst. of Tech., Pasadena, CA USA Graphic Three-Axes Presentation of Residual Gas Analyzer Data

Johnson, Kenneth R., Jet Propulsion Lab., California Inst. of Tech., USA; Levi, Alejandro G., Jet Propulsion Lab., California Inst. of Tech., USA; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 355-361; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Residual gas analyzers (RGA) are commonly used to measure the composition of residual gases in thermal-vacuum test chambers. Measurements from RGA's are often used to identify and quantify outgassing contaminants from a test article during thermal-vacuum testing. RGA data is typically displayed as snapshots in time, showing instantaneous concentrations of ions from ionized residual gas molecules at different atomic masses. This ion concentration information can be interpreted to be representative of the composition of the residual gas in the chamber at the instant of analysis. Typically, test personnel are most interested in tracking the time history of changes in the composition of chamber residual gas to determine the relative cleanliness and the clean-up rate of the test article under vacuum. However, displays of instantaneous RGA data cannot provide test personnel with the preferred time history information. In order to gain an understanding of gas composition trends, a series of plots of individual data snapshots must be analyzed. This analysis is cumbersome and still does not provide a very satisfactory view of residual gas composition trends. A method was devised by the authors to present RCA data in a three-axis format, plotting Atomic Mass Unit (AMU), the Ionization Signal Response (ISR) as

amps/torr as a function of AMU, and Time, to provide a clear graphic visualization of trends of changes in ISR with respect to time and AMU (representative of residual gas composition). This graphic visualization method provides a valuable analytical tool to interpret test article outgassing rates during thermal vacuum tests. Raw RGA data was extracted from a series of delimited ASCII files and then converted to a data array in a spreadsheet. Consequently, using the 3-D plotting functionality provided by the spreadsheet program, 3-D plots were produced. After devising the data format conversion process, the authors began developing a program to provide real-time 3-D plotting of RGA data. The intent of this program is to automate the RGA data acquisition process and to generate up-to-the-minute time history 3-D displays of stored RGA data (development of this program was not complete at the time of this writing). This paper provides a brief description of the data format conversion process and presents results from a recent test to illustrate the usefulness of this 3-D RGA data plotting technique.

Author

Computer Graphics; Three Dimensional Models; Residual Gas; Gas Composition; Gas Analysis; Ionized Gases; Ion Concentration

19970020065 New Orleans Univ., Dept. of Chemistry, LA USA

Computed Heats of Formation of Three Tetraazapentalenes, A Tris(Nitrotriazolo)Triazine, and a Tricyclic Gem-Difluor-Amino/Tetranitramine

Politzer, Peter, New Orleans Univ., USA; Grice, M. E., New Orleans Univ., USA; Murray, Jane S., New Orleans Univ., USA; Nov. 14, 1996; 4p; In English

Contract(s)/Grant(s): N00014-97-I-0066

Report No.(s): AD-A319355; TR-97; No Copyright; Avail: CASI; A01, Hardcopy; A01, microfiche

We have used our density functional procedure to compute the heats of formation of the compounds 1-5. The vibrational energies were determined from the molecular stoichiometries. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface. DTIC

Heat of Formation; Organic Compounds

19970020216 California Univ., Davis, CA USA

Experiments in Turbulent Spray Combustion Final Report, 15 Jun. 1992 - 14 Jun. 1996

Kennedy, Ian M., California Univ., USA; Lienau, Jeffrey, California Univ., USA; Aug. 21, 1996; 3p; In English Contract(s)/Grant(s): F49620-92-J-0364; AF Proj. 3484

Report No.(s): AD-A315719; AFOSR-96-0441TR; No Copyright; Avail: CASI; A01, Hardcopy; A01, microfiche

A major part of the research effort during the period of the AASERT award was the re-design of a system to produce a spray of liquid in a well defined simple geometry. Loadings of about 50% were obtained with the new system. Measurements of the dispersion of tagged fluorescent particles were obtained by filtering the intense Mie scattering with a combination of colored glass and holographic filters. The measurements showed that the presence of the dispersed phase had a strong impact on the particle dispersion. The graduate students who were assigned to this project gained valuable experience in turbulent two phase fluid mechanics, optics and laser diagnostics as they were involved in assembling the droplet measurement system.

Turbulent Combustion; Flow Visualization; Fluorescence; Mie Scattering; Drops (Liquids); Sprayers

19970020218 Northwestern Univ., Dept. of Materials Science and Engineering, Evanston, IL USA

Nanostructure of Au-2O% Pd Layers in MoS2 Multilayer Solid Lubricant Films

Jayaram, G., Northwestern Univ., USA; Marks, L. D., Northwestern Univ., USA; Hilton, M. R., Aerospace Corp., USA; Jun. 01, 1996; 13p; In English; Sponsored in part by the Aerospace Sponsored Research program.

Contract(s)/Grant(s): F49620-94-I-0164

Report No.(s): AD-A316374; ATR-95(8561)-1; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

High-resolution electron microscopy imaging and electron and X-ray diffraction techniques have been used to characterize the structure of low and high flux Au-20%Pd layers in Au-20%Pd/MoS2 multilayer solid lubricant thin films. Images clearly reveal different morphologies for the metal layers in the two flux regimes, which can be correlated to the variation in fracture resistance reported by an earlier indentation study. In the lower metal flux regime, three-dimensional islands with single-crystal and multiply twinned structures are seen, while quasi-continuous, polycrystalline regions are seen in the higher flux case.

DTIC

Solid Lubricants; Thin Films; Microstructure; Fracture Strength; Gold Alloys; Palladium Alloys; Molybdenum Disulfides; Imaging Techniques

19970020222 Northwestern Univ., Dept. of Chemistry, Evanston, IL USA

Energetics of Electron Transfer at the Nanocrystalline Titanium Dioxide Semiconductor/Aqueous Solution Interface: pH Invariance of the Metal Based Formal Potential of a Representative Surface Attached Dye Couple

Yan, Susan G., Northwestern Univ., USA; Hupp, Josep T., Northwestern Univ., USA; Oct. 1996; 15p; In English Contract(s)/Grant(s): N00014-91-J-1035

Report No.(s): AD-A316894; TR-34; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Mediator-based spectroelectrochemical assessment of the metal-centered formal potential (E sub f(RU)) of a representative inorganic dye, Ru(4,4'-(CH2PO3)-2,2'-bipyridine)(sub 3)(sup 10-), bound to a nanocrystalline titanium dioxide film shows that the potential is insensitive to changes in solution pH, despite significant shifts in the conduction band edge energy (E (sub CB)) of the underlying semiconductor electrode in response to the same environmental perturbations. The observations are important in the context of recent work showing that back electron reactivity for the same semiconductor/dye combination is pH independent over a 19 pH unit range, despite apparent changes in back reaction driving force of greater than 1.2 eV over the same interval (Yan, S.; Hupp, J. T. J Phys. Chem. 1996, 100, 6867). In particular, the spe ctroelectrochemical findings serve to rule out a suggested alternative interpretation of the unusual kinetic effects whereby the crucial energy difference quantity, E(sub CB) - E(sub f)(sup RU), remains fixed because of compensating changes in the dye potential with pH.

Semiconductor Devices; Electron Transfer; Energy Conversion Efficiency; Titanium Oxides; pH

#### 19970020295 Naval Research Lab., Washington, DC USA

# Upward Flame Spread on Vertical Surfaces Interim Report, Mar. 1995 - Mar 1996

Williams, F. W., Naval Research Lab., USA; Beyler, C. L., Hughes Associates, Inc., USA; Hunt, S. P., Hughes Associates, Inc., USA; Iqbal, N., Hughes Associates, Inc., USA; Jan. 13, 1997; 70p; In English; Limited Reproducibility: More than 20% of this Document may be affected by microfiche quality

Report No.(s): AD-A320757; NRL/MR/6180--97-7908; No Copyright; Avail: Issuing Activity (Defense Technical Information Center (DTIC)), microfiche

A model which describes the physical processes of upward flame spread and for growth on wall materials has been developed and implemented as a computer program. The computer based flame spread model simulates the fire growth along a vertical combustible wall. The vertical wall material may be heated by an imposed external heat flux and is ignited at its bottom edge with a flame from a line burner of user specified strength. The model predicts the flame spread rate, the heat release rate of the fire, the flame height, the net heat flux to the wall surface and the time varying surface temperatures. The model uses inputs developed from cone calorimeter data. The results from the model compare favorably to experimental upward flame spread results for polymethylmethacrylate, plywood and wood particle board found in the literature. The sensitivity of the model to material thermal properties, flame heat flux and flame height are systematically examined.

Flame Propagation; User Manuals (Computer Programs); Computer Programs; Thermodynamic Properties; Heat Transfer

19970020297 Hawaii Univ., Dept. of Physics and Astronomy, Honolulu, HI USA

#### Atomic Hydrogen Trapped in Solid H2 Final Report

Gaines, James R., Hawaii Univ., USA; Sep. 1996; 56p; In English

Contract(s)/Grant(s): F29601-92-K-0013; AF Proj. 3058

Report No.(s): AD-A317268; PL-TR-95-3036; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

The technical work under this contract focused on production and storage of hydrogen atoms in molecular hydrogen hosts. Studies of the diffusion of molecules and atoms in hydrogen hosts were made. In crystalline solids D is controlled by the number of vacancies in the lattice. Values of the parameters used for theory were obtained for all isotopes. Data for the isotopes can be successfully scaled by the quantum parameter. The atom and molecule hop frequencies were found to be almost identical, making possible the prediction of atom recombination rates. Isotropic substitution has the same effect on the diffusion as increased pressure, but recombination coefficients for crystalline and amorphous solids differ. The anomalous atom growth curves in titrated solids were explained, and a method, based on filling the solid's vacancies, was found for obtaining large atom densities. A new model for in situ atom production for solids containing tritium was developed. Experiments yielding the diffusion coefficient of HD and H2 molecules absorbed on activated carbon fibers indicate that these fibers are effective catalysts of the ortho-para transition. Three suggestions are made for future investigation.

**DTIC** 

Atoms; Hydrogen Atoms; Atomic Structure; Solidified Gases

19970020316 Air Force Inst. of Tech., Wright-Patterson AFB, OH USA

# Laser-Induced Breakdown Spectroscopy on Solution Samples Using Surface Excitation

Berman, Leonard M., Air Force Inst. of Tech., USA; Dec. 1996; 112p; In English

Report No.(s): AD-A320544; AFIT/GAP/ENP/96D-03; No Copyright; Avail: CASI; A06, Hardcopy; A02, microfiche

Laser-induced breakdown spectroscopy (LIBS) is a spectroscopic technique where output from a pulsed laser is focused onto a target in order to create an intense plasma. The optical emission is characteristic of the elements in the focal volume and can be used for elemental analysis. Research on the detection of nickel in solution in addition to solvent detection of CCl4, CHCl3, C2Cl4, and C2HCl3 has been performed. Breakdown was formed at the sample surface via a Q-switched Nd:YAG laser. Initially, operation of the laser was at 1064 nm/repetition rate of 5 Hz. Experiments were also performed using the third harmonic (355 nm)/repetition rate of 20 Hz. Pulse energy was maintained at 60 mJ. The spark light was spectrally resolved and detected by a time-gated photodiode array. A 50 microsecond gate width/8 microsecond time delay gave detection limits of 56.1 mg/l for nickel in solution. In the UV, a 10 microsecond gate width/3 microsecond time delay lowered detection limits down to 29.4 mg/l. Concentrations spanned from 50 to 1000 mg/l. Using UV excitation (10 microsecond gate width/l microsecond time delay), saturated solvent solutions as high as 7.71 g/l were not detectable.

**DTIC** 

Pulsed Lasers; YAG Lasers; Q Switched Lasers; Spectroscopy; Light Emission; Environmental Monitoring; Laser Applications

#### 19970020549 Massachusetts Inst. of Tech., Cambridge, MA USA

#### Fullerenes, PAH, Carbon Nanostructures, and Soot in Low Pressure Diffusion Flames

Grieco, William J., Massachusetts Inst. of Tech., USA; Lafleur, Arthur L., Massachusetts Inst. of Tech., USA; Rainey, Lenore C., Massachusetts Inst. of Tech., USA; Taghizadeh, Koli, Massachusetts Inst. of Tech., USA; VanderSande, John B., Massachusetts Inst. of Tech., USA; Howard, Jack B., Massachusetts Inst. of Tech., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 13-18; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1879; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The formation of fullerenes C60 and C7O is known to occur in premixed laminar benzene/oxygen/argon flames operated at reduced pressures. High resolution transmission electron microscopy (HRTEM) images of material collected from these flames has identified a variety of multishelled nanotubes and fullerene 'onions' as well as some trigonous structures. These fullerenes and nanostructures resemble the material that results from commercial fullerene production systems using graphite vaporization. As a result, combustion is an interesting method for fullerenes synthesis. If commercial scale operation is to be considered, the use of diffusion flames might be safer and less cumbersome than premixed flames. However, it is not known whether diffusion flames produce the types and yields of fullerenes obtained from premixed benzene/oxygen flames. Therefore, the formation of fullerenes and carbon nanostructures, as well as polycyclic aromatic hydrocarbons (PAH) and soot, in acetylene and benzene diffusion flames is being studied using high performance liquid chromatography (HPLC) and high resolution transmission electron microscopy (HRTEM).

Derived from text

Diffusion Flames; Premixed Flames; Combustion Chemistry; Soot; Polycyclic Aromatic Hydrocarbons; Fullerenes; Fuel Combustion; Carbon; Microstructure; Combustion Products

# 19970020553 Washington Univ., Saint Louis, MO USA

# **Gas-Phase Combustion Synthesis of Metal and Ceramic Nanoparticles**

Axelbaum, R. L., Washington Univ., USA; Chao, B. H., Hawaii Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 37-42; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Gas-phase combustion (flame) synthesis has been an essential industrial process for producing large quantities of powder materials such as carbon black, titanium dioxide, and silicon dioxide. Flames typically produce simple oxides, with carbon black being the noted exception because the oxides of carbon are gaseous and are easily separated from the particulate matter that is formed during fuel pyrolysis. The powders produced in flames are usually agglomerated, nanometer-sized particles (nanoparticles). This is an acceptable composition and morphology for many applications. However, recently there has been interest in flames for the synthesis of metal and non-oxide ceramic unagglomerated nanoparticles (2 to 100 nm) for advanced materials applications. For these applications nano-powders are consolidated into bulk materials under high temperature and pressure, yielding a solid part whose grains retain the nanometer size of the starting powder. The final nanostructured materials often possess

unique mechanical, electrical or magnetic properties compared to their coarse-grained counterparts. The economics of powder processing can also be enhanced with nano-powders vis-a-vis low temperature consolidation and superplastic forming.

Derived from text

Combustion Synthesis; Vapor Phases; Ceramics; Powder Metallurgy; Crystal Structure; Flames; Superplastic Forming; Synthesis (Chemistry); Particulates

#### 19970020555 AeroChem Research Labs., Inc., Princeton, NJ USA

#### **Internal and Surface Phenomena in Heterogenous Metal Combustion**

Dreizin, Edward L., AeroChem Research Labs., Inc., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 49-54; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAS3-27259; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The phenomenon of gas dissolution in burning metals was observed in recent metal combustion studies, but it could not be adequately explained by the traditional metal combustion models. The research reported here addresses heterogeneous metal combustion with emphasis on the processes of oxygen penetration inside burning metal and its influence on the metal combustion rate, temperature history, and disruptive burning. The unique feature of this work is the combination of the microgravity environment with a novel micro-arc generator of monodispersed metal droplets, ensuring repeatable formation and ignition of uniform metal droplets with a controllable initial temperature and velocity. Burning droplet temperature is measured in real time with a three wavelength pyrometer. In addition, particles are rapidly quenched at different combustion times, cross-sectioned, and examined using SEM-based techniques to retrieve the internal composition history of burning metal particles. When the initial velocity of a spherical particle is nearly zero, the microgravity environment makes it possible to study the flame structure, the development of flame nonsymmetry, and correlation of the flame shape with the heterogeneous combustion processes.

Derived from text

Metal Combustion; Reaction Kinetics; Combustion Chemistry; Oxygen; Microgravity; Heterogeneity; Metals

#### 19970020556 AeroChem Research Labs., Inc., Princeton, NJ USA

#### **Interaction of Burning Metal Particles**

Dreizin, Edward L., AeroChem Research Labs., Inc., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 55-60; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAS3-96017; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Multiple particle/droplet flames are ubiquitous in practical combustion systems, and thus the flame interaction processes are of great practical importance. This explains the strong current interest in interactive combustion phenomena. This research is aimed at the investigation of combustion parameters of microgravity model aerosols: relatively large uniform metal particles aerosolized in microgravity environment. An experiment consisting of creation and ignition of a metal multiparticle system in microgravity and high-speed video-recording of the combustion events will produce visual records of the development of individual particle flames, their interactions and the particle motion they induce simultaneously with the observation of the entire aerosol combustion process. Frame by frame analysis of the video-images taken using a high-speed movie camera will allow one to determine particle brightness temperatures and the decrease in particle diameter during combustion. Analysis of the experimental results and comparison with the results of single metal particle combustion experiments, conducted under similar microgravity conditions in the framework of a parallel program, will establish the relationship between single and multiple particle burning rates and combustion temperatures, concentrations at which the flame substructure forms rather than individual particle flames, efficiency of radiative heat transfer in metal aerosol combustion, what is the role of electrostatic forces in structuring the flame and the effect of that structure on the flame propagation rate. Although some details of fine particle aerosol clouds, such as the kinetics limited burning rate, radiative heat transfer in a system with a high specific surface, particle induced turbulence, etc., will probably not be very well simulated in the planned experiments, they are relatively well understood and can be accounted for using an adequate individual particle combustion model. On the other hand, the unknown particle interaction phenomena to be studied in this research program are generic and can be readily projected onto a cloud combustion model which would also incorporate a correction for particle size.

Derived from text

Metal Particles; Metal Combustion; Flames; Combustion Physics; Chemical Reactions; Burning Rate; Aerosols; Microgravity; Drops (Liquids)

19970020559 Northwestern Univ., School of Engineering and Applied Science, Evanston, IL USA Spherical Diffusion Flames: Structure and Dynamics

Matalon, Moshe, Northwestern Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 75-80; In

English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1604; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The spherical geometry is the most suitable one to study fundamental issues concerning the structure and the dynamics of diffusion flames. From a theoretical point of view, it is the only geometry that permits the existence of a truly one dimensional stationary diffusion flame. A stationary planar diffusion flame with the fuel supplied upstream, at x approaches -infinity say, and the oxidant downstream, at x approaches +infinity is not possible. For a steady diffusion flame to exist, one must have nonzero fluxes of fuel and oxidant towards the flame. However, in the unlimited region behind the planar flame the only bounded solutions to the reaction-free convective-diffusive operator are constants. Hence the oxidant concentration behind the flame remains constant and there is no mechanism to generate the necessary flux towards the flame. A one-dimensional problem can be formulated if the reactants are supplied at finite locations; but the boundary conditions in this case introduce unnecessary complications and do not appropriately model the physical reality. Indeed, a planar diffusion flame can be established in the stagnation-point flow of two opposed jets but the flame in this case is stretched and the flow is essentially two-dimensional. The only stationary one-dimensional diffusion flame in an unlimited environment is therefore the spherical flame.

Derived from text

Diffusion Flames; Boundary Layer Combustion; Jet Flow; Burning Rate; Combustion Physics; Flame Propagation; Flame Stability; Fuel Combustion

#### 19970020560 Northwestern Univ., Dept. of Mechanical Engineering, Evanston, IL USA

# Reactive Hydrodynamics in Rotating Spherical and Cylindrical Geometry

Sohrab, Siavash H., Northwestern Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 81-86; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1863; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

In turbulent spray combustion among many complex interactions between local flow structures called turbulent eddies and droplets are those associated with rotation of droplets. In general, for a complete statistical description of turbulent sprays, consideration of at least four degrees of freedom respectively associated with translational, rotational, vibrational (pulsational), and internal motions of the droplet are needed. Clearly the interactions between all degrees of freedom of the droplets and those for the gaseous background field will be exceedingly complex. For example, one type of interaction between the translational and the rotational velocity of droplets results in droplet helicity,  $H(d) = w(d) \cdot v(d)$ , the significance of which in turbulent spray combustion is yet to be recognized. The role of droplet rotation in turbulent spray combustion modeling and its impact on the evaporation of liquid fuel droplets was recently investigated. Also, the impact of rotation on combustion of solid particles such as is encountered in pulverized coal combustion has been emphasized. The problem of viscous flow around a rotating sphere discussed above also occurs in other areas of physical sciences such as astrophysics and geophysics. Consequently, the subject has been addressed in many classical as well as more recent investigations. According to these investigations, the rotation of a rigid sphere in an otherwise quiescent, unconfined environment results in the motion of the fluid towards the poles. The polar flows from the northern and southern hemispheres move along helical trajectories towards the equatorial plane. Eventually, the polar flows collide at the equatorial plane, thus producing a sheet of rotating fluid that is radially ejected outward on this plane. Therefore, a droplet induces a strained flow field as a result of its rotation. Since the spatial extent of equatorial jets could easily exceed many droplet diameters, interactions between neighboring droplets are enhanced as a result of their rotation. Also, the equatorial jet substantially alters the spherical geometry of the diffusion flame surface that surrounds a rotating droplet. The objective of the research is to gain more knowledge about the hydrodynamics within and around rotating spherical and cylindrical body of fluid, and the behavior of diffusion or premixed flame surfaces that could surround such symmetric body of rotating fluid.

Derived from text

Cylindrical Bodies; Combustion Chemistry; Diffusion Flames; Hydrodynamics; Liquid Fuels; Premixed Flames; Reaction Kinetics; Rotating Spheres; Turbulent Combustion; Viscous Flow

# 19970020561 Maryland Univ., Dept. of Fire Protection Engineering, College Park, MD USA Diffusion Flame Extinction in a Low Strain Flow

Sutula, Jason, Maryland Univ., USA; Jones, Joshua, Maryland Univ., USA; Torero, Jose L., Maryland Univ., USA; Borlik, Jeffrey, Texas Univ., USA; Ezekoye, Ofodike A., Texas Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 87-92; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Diffusion flames are of great interest in fire safety and many industrial processes. Many parameters significantly affect the flame structure, shape and stability, of particular importance are the constraints imposed by geometrical boundaries. Physical boundaries determine the characteristics of the flow, affect heat, fuel, and oxidizer transport from and towards the flame and can act as heat sinks or heat sources. As a result, the existence of a flame, its shape and nature are intimately related to the geometrical

characteristics of the environment that surrounds it. The counter-flow configuration provides a constant strain flow, therefore, is ideal to study the structure of diffusion flames. Most studies have concentrated on the high velocity, high strain limit, since buoyantly induced instabilities will disintegrate the planar flame as the velocity decreases. Only recently, experimental studies in micro-gravity conditions have begun to explore the low strain regimes. The main objective of these on-going studies is to determine the effect of radiative heat losses and variable strain on the structure and radiation-induced extinction of diffusion flames. For these programs, size, geometry, and experimental conditions have been chosen to keep the flame unaffected by the physical boundaries. Whether is the burning of condensed or gaseous fuels, for most real situations the boundaries impose a significant effect on the nature of the flame. There is, therefore, a need to better understand the effect that geometrical constraints (i.e. flow nonperpendicular to a fuel surface, heat losses to the boundaries, etc.) might have on the final characteristics of a diffusion flame. Preliminary experiments have shown that, in the absence of gravity, and depending on the distance from the flame to the boundary, three characteristically different regimes can be observed. Close to the boundary, the flame is parabolic, very thin and blue, almost soot-less. Diffusion is the main mechanism controlling fuel transport to the reaction zone, conduction towards the inlets is the main source of heat losses. As the distance increases the flame becomes linear and thickens, remaining blue at the oxidizer side and turning yellow at the fuel side. Here, convection brings fuel and oxidizer together and the reaction occurs in the viscous layer formed between the fuel and oxidizer streams. This region corresponds to the characteristic counter-flow flame where conduction and convection become negligible forms of heat losses and radiation becomes dominant. The flame in the third (mixed) region, between the two others, results from the combination of the scenarios presented above.

Derived from text

Diffusion Flames; Flame Stability; Microgravity; Oxidizers; Fuel Combustion; Diffusion; Gaseous Fuels

#### 19970020562 NASA Lewis Research Center, Cleveland, OH USA

#### Strain-Rate-Free Diffusion Flames: Initiation, Properties, and Quenching

Fendell, Francis, TRW Space and Electronics Group, USA; Rungaldier, Harald, TRW Space and Electronics Group, USA; Gokoglu, Suleyman, NASA Lewis Research Center, USA; Schultz, Donald, NASA Lewis Research Center, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 93-98; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAS3-27264; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

For about a half century, the stabilization of a steady planar deflagration on a heat-sink-type flat-flame burner has been of extraordinary service for the theoretical modeling and diagnostic probing of combusting gaseous mixtures. However, most engineering devices and most unwanted fire involve the burning of initially unmixed reactants. The most vigorous burning of initially separated gaseous fuel and oxidizer is the diffusion flame. In this useful idealization (limiting case), the reactants are converted to product at a mathematically thin interface, so no interpenetration of fuel and oxidizer occurs. This limit is of practical importance because it often characterizes the condition of optimal performance (and sometimes environmentally objectionable operation) of a combustor. A steady planar diffusion flame is most closely approached in the laboratory in the counterflow apparatus. The utility of this simple-strain-rate flow for the modeling and probing of diffusion flames was noted by Pandya and Weinberg 35 years ago, though only in the last decade or so has its use become internationally common place. However, typically, as the strain rate a is reduced below about 20 cm(exp -1), and the diffusion-flame limit (reaction rate much faster than the flow rate) is approached, the burning is observed to become unstable in earth gravity. The advantageous steady planar flow is not available in the diffusion-flame limit in earth gravity. This is unfortunate because the typical spatial scale in a counterflow is (k/a)(sup 1/2), where k denotes a characteristic diffusion coefficient; thus, the length scale becomes large, and the reacting flow is particularly amenable to diagnostic probing, as the diffusion-flame limit is approached. The disruption of planar symmetry is owing the fact that, as the strain rate a decreases, the residence time (1/a) of the throughput in the counterflow burner increases. Observationally, when the residence time exceeds about 50 msec, the inevitably present convective (Rayleigh-Benard) instabilities, associated with hot-under-cold (flame-under-fresh-reactant) stratification of fluid in a gravitational field, have time to grow to finite amplitude during transit of the burner.

Derived from text

Diffusion Flames; Initiation; Heat Sinks; Gaseous Fuels; Gas Mixtures; Combustion; Combustion Chambers; Counterflow; Burners; Oxidizers; Reacting Flow; Reaction Kinetics; Strain Rate; Stratification

# 19970020563 Centre National de la Recherche Scientifique, Lab. de Combustion, Paris, France

# Experimental Study on the Stability of a Diffusion Flame Established in a Laminar Boundary Layer

Brahmi, Lynda, Centre National de la Recherche Scientifique, France; Vietoris, Thomas, Centre National de la Recherche Scientifique, France; Joulain, Pierre, Centre National de la Recherche Scientifique, France; Torero, Jose L., Maryland Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 99-103; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

A series of normal gravity and micro-gravity experiments have been conducted to study the blow-off limits of a laminar diffusion flame. The effect of gravity was evaluated by placing the fuel surface above and below the oxidizer stream. It was observed that blow-off limits in ceiling and floor configuration differ in a qualitative way but blow-off occurs at very similar oxidizer and fuel velocities. In micro gravity, the flame is significantly more stable and although no clear blow-off limits could be determined, four characteristic flame regimes were identified. The use of IR thermography to obtain flame temperatures has been proven to be feasible.

Derived from text

Diffusion Flames; Convective Flow; Combustion; Flame Propagation; Gaseous Fuels; Laminar Boundary Layer; Multiphase Flow; Surface Diffusion; Turbulent Flow; Microgravity; Gravitational Effects; Laminar Flow

#### 19970020564 Tohoku Univ., Inst. of Fluid Science, Sendai, Japan

#### **Radiative Extinction of Counterflow Premixed Flames**

Maruta, Kaoru, Tohoku Univ., Japan; Ju, Yi-Guang, Tohoku Univ., Japan; Guo, Hong-Sheng, Tohoku Univ., Japan; Niioka, Takashi, Tohoku Univ., Japan; Fourth International Microgravity Combustion Workshop; May 1997, pp. 105-110; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

This report presents experiments on counterflow premixed flames at small stretch rates and relevant numerical calculation involving radiation loss from the flame zone. Extinction experiments on counterflow methane/air and propane/air premixed flames at small stretch rates are conducted under microgravity to observe extinction characteristics of near-limit premixed twin flames. The results show two kinds of flame response, that is, C-shaped extinction curve due to radiative loss for methane/air mixture and ordinal monotonous extinction curve for propane/air mixture. to analyze these experiments, numerical investigation addressing extinction and flammable regions of radiative counterflow premixed flames for Lewis numbers from unity to 1.82 are conducted to clarify the mechanism of these two kinds of flame response. The computation exhibited flame bifurcation resulting in a G-shaped extinction curve showing the extended limit of flammability for Lewis number near unity and a K-shaped extinction curve showing the composition flammability limit being equal to that of one-dimensional flame for Lewis number of 1.82. G-and K-shaped extinction curves respectively explain the experimental C curve for methane/air and monotonous curve for propane/air mixtures. Furthermore, the relationship between the composition flammability limit of one dimensional propagating flame and that of stretched flames is clarified.

Author

Counterflow; Premixed Flames; Gas Mixtures; Flammability; Microgravity; Fuel Combustion

### 19970020565 NASA Lewis Research Center, Cleveland, OH USA

# Structure and Stability of Burke-Schumann Diffusion Flames

Lee, Yong G., Iowa Univ., USA; Chen, Lea-Der, Iowa Univ., USA; Brooker, John E., NASA Lewis Research Center, USA; Stocker, Dennis P., NASA Lewis Research Center, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 111-116; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1592; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The general goal of this NASA Grant is twofold: to improve our understanding of (1) the influence of buoyancy on the stability and structure of Burke-Schumann type diffusion flames, and (2) the effects of buoyancy on vortex-flame interactions in co-flow diffusion flames. A numerical code with a higher order accuracy for spatial discretization is developed in this project for simulation of time-dependent diffusion flames by Sheu and Sheu and Chen, and an extended reduced mechanism is incorporated for prediction of methane oxidation and NO(x)(NO, NO2, and N2O) formation and emission from methane Burke-Schumann diffusion flame (BSDF) as reported in Sheu, and Sheu and Chen. Initial investigation of vortex and flame interaction within the context of fast chemistry is reported. Experiments are conducted in reduced pressure to study the lift-off and stabilization of methanefueled BSDF in reduced buoyancy environments due to reduced pressure. Measurements of temperature and species concentrations are made in normal and reduced pressure environments to study the effects of buoyancy on the structure of BSDF, and will be reported in this paper. to study the buoyancy effects on the lift-off and stabilization of methane-fueled jet diffusion flames in coflowing air, a glovebox investigation, Enclosed Laminar Flames (ELF), has been proposed and approved for space-based testing on the fourth USA Microgravity Payload (USMP-4) mission, scheduled for October 1997. A brief description of the ELF investigation is also presented.

Derived from text

Diffusion Flames; Buoyancy; Flame Propagation; Laminar Flow; Microgravity; Flame Stability; Fuel Combustion; Jet Flow

#### 19970020566 NASA Lewis Research Center, Cleveland, OH USA

#### Study of Buoyancy Effects in Diffusion Flames Using Rainbow Schlieren Deflectometry

Agrawal, Ajay K., Oklahoma Univ., USA; Gollahalli, Subramanyam R., Oklahoma Univ., USA; Griffin, DeVon, NASA Lewis Research Center, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 117-122; In English; Also announced as 19970020547; Original contains color illustrations

Contract(s)/Grant(s): NAG3-1594; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Diffusion flames are extensively encountered in many domestic and industrial processes. Even after many decades of research, a complete understanding of the diffusion flame structure is not available. The structure and properties of the flames are governed by the mixing (laminar or turbulent), chemical kinetics, radiation and soot processes. Another important phenomenon that affects flame structure in normal gravity is buoyancy. The presence of buoyancy has long hindered the rational understanding of many combustion processes. In gas jet diffusion flames, buoyancy affects the structure of the shear layer, the development of fluid instabilities, and formation of the coherent structures in the near nozzle region of the gas jets. The buoyancy driven instabilities generate vorticial structures outside the flame resulting in flame flicker. The vortices also strongly interact with the small-scale structures in the jet shear layer. This affects the transitional and turbulence characteristics of the flame. For a fundamental understanding of diffusion flames it is essential to isolate the effects of buoyancy. This is the primary goal of the experiments conducted in microgravity. Previous investigations, have shown dramatic differences between the jet flames in microgravity and normal gravity. It has been observed that flames in microgravity are taller and more sooty than in normal gravity. The fuels used in these experiments were primarily hydrocarbons. In the absence of buoyancy the soot resides near the flame region, which adversely affects the entrainment of reactants. It is very important to eliminate the interference of soot on flame characteristics in microgravity. The present work, therefore, focuses on the changes in the flame structure due to buoyancy without the added complexities of heterogeneous reactions. Clean burning hydrogen is used as the fuel to avoid soot formation and minimize radiative losses. Because of the low luminosity of hydrogen flames, we use rainbow schlieren deflectometry for visualization. The visualized images are digitized for quantification. The work reported here is divided into three sections; rainbow schlieren deflectometry (RSD), microgravity experiments and sub-atmospheric pressure experiments. The first section demonstrates the application of RSD for quantitative measurements in non-reacting and reacting flow systems. A computational effort to complement the experimental work is also included. In the second section, the experiments conducted at the 2.2s NASA Lewis Drop tower facility are described. The experiments were conducted to study the behavior of laminar, transitional and turbulent hydrogen flames in microgravity. The ability of RSD technique to provide quantitative data is highlighted. The final section deals with the sub-atmospheric pressure tests, which demonstrate that buoyancy in hydrogen diffusion flames can be scaled with pressure at normal gravity. Derived from text

Buoyancy; Diffusion Flames; Combustion Physics; Deflection; Microgravity; Jet Flow; Turbulence; Gas Jets; Fuels

### 19970020568 NASA Lewis Research Center, Cleveland, OH USA

### Shapes of Buoyant and Nonbuoyant Methane Laminar Jet Diffusion Flames

Sunderland, Peter B., National Academy of Sciences - National Research Council, USA; Yuan, Zeng-Guang, NYMA, Inc., USA; Urban, David L., NASA Lewis Research Center, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 129-134; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Laminar gas jet diffusion flames represent a fundamental combustion configuration. Their study has contributed to numerous advances in combustion, including the development of analytical and computational combustion tools. Laminar jet flames are pertinent also to turbulent flames by use of the laminar flamelet concept. Investigations into the shapes of noncoflowing microgravity laminar jet diffusion flames have primarily been pursued in the NASA Lewis 2.2-second drop tower, by Cochran and coworkers and by Bahadori and coworkers. These studies were generally conducted at atmospheric pressure; they involved soot-containing flames and reported luminosity lengths and widths instead of the flame-sheet dimensions which are of Greater value to theory evaluation and development. The seminal model of laminar diffusion flames is that of Burke and Schumann, who solved the conservation of momentum equation for a jet flame in a coflowing ambient by assuming the velocity of fuel, oxidizer and products to be constant throughout. Roper and coworkers improved upon this model by allowing for axial variations of velocity and found flame shape to be independent of coflow velocity. Roper's suggestion that flame height should be independent of gravity level is not supported by past or present observations. Other models have been presented by Klajn and Oppenheim, Markstein and De Ris, Villermaux and Durox, and Li et al. The common result of all these models (except in the buoyant regime) is that flame height is proportional to fuel mass flowrate, with flame width proving much more difficult to predict. Most existing flame models have been compared with shapes of flames containing soot, which is known to obscure the weak blue emission of flame sheets. The present work involves measurements of laminar gas jet diffusion flame shapes. Flame images have been obtained for buoyant and nonbuoyant methane flames burning in quiescent air at various fuel flow-rates, burner diameters and ambient pressures. Soot concentrations were minimized by selecting conditions at low flowrates and low ambient pressures; this allows identification of actual flame sheets associated with blue emissions of CH and CO2. The present modeling effort follows that of Roper and is useful in explaining many of the trends observed.

Derived from text

Diffusion Flames; Buoyancy; Gas Jets; Laminar Flow; Methane; Microgravity; Fuel Combustion; Jet Flow; Shapes

# 19970020569 Colorado Univ., Center for Combustion Research, Boulder, CO USA

#### **Splitting of Forced Elliptic Jets and Flames**

Hertzberg, J., Colorado Univ., USA; Carlton, J., Colorado Univ., USA; Schwieterman, M., Colorado Univ., USA; Davis, E., Colorado Univ., USA; Bradley, E., Colorado Univ., USA; Linne, M., Colorado School of Mines, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 135-140; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1616; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The objective of this work is to understand the fluid dynamics in the interaction of large scale, three-dimensional vortex structures and transitional diffusion flames in a microgravity environment. The vortex structures are used to provide a known perturbation of the type used in passive and active shear layer control techniques. 'Passive techniques' refers to manipulation of the system geometry to influence the three dimensional dynamics of vortex structures, and 'active' refers to any technique which adds energy (acoustic or kinetic) to the flow to influence the shear layer vortex dynamics. In this work the passive forcing is provided by an elliptic jet cross-section, and the active forcing is incorporated by perturbing the jet velocity using a loudspeaker in the plenum section.

Derived from text

Diffusion Flames; Microgravity; Loads (Forces); Diffusion; Jet Flow; Flow Visualization; Vortices; Perturbation

# 19970020570 Massachusetts Inst. of Tech., Cambridge, MA USA

# Application of Shear Plate Interferometry to Jet Diffusion Flame Temperature Measurements

VanDerWege, Brad A., Massachusetts Inst. of Tech., USA; OBrien, Chris J., Massachusetts Inst. of Tech., USA; Hochgreb, Simone, Massachusetts Inst. of Tech., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 141-144; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-160; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The recent ban on the production of bromotrifluoromethane (CF3Br) because of its high stratospheric ozone depletion potential has led to interest in finding alternative agents for fire extinguishing applications. Some of the promising alternatives are fluorinated hydrocarbons. A clear understanding of the effects of CF3Br and alternative chemical suppressants on diffusion flames is therefore necessary in the selection of alternative suppressants for use in normal and microgravity. The flame inhibition effects of halogen compounds have been studied extensively in premixed systems. The effect of addition of halocarbons (carbon-halogen compounds) to diffusion flames has been studied experimentally in coflow configurations and in counterflow gaseous and liquidpool flames. Halogenated compounds are believed to inhibit combustion by scavenging hydrogen radicals to form the relatively unreactive compound HF, or through a catalytic recombination cycle involving HBr to form H2. Comparisons between halogens show that bromine inhibition is significantly more effective than chlorine or fluorine. Although fluorinated compounds are only slightly more effective inhibitors on a mass basis than nitrogen, they are more effective on a volume basis and are easily stored in liquid form. The objectives of this study are (a) to determine the stability limits of laminar jet diffusion flames with respect to inhibitor concentration in both normal and microgravity, and (b) to investigate the structure of halocarbon-inhibited flames. In the initial phase of this project, visual diagnostics were used to observe the structure and behavior of normal and microgravity flames. The initial observations showed significant changes in the structure of the flames with the addition of halocarbons to the surrounding environment, as discussed below. Furthermore, the study established that the flames are more stable relative to the addition of halocarbons in microgravity than in normal gravity. Visual diagnostics of flames are, however, necessarily limited to detection of radiative emission in the visible range, and offer only qualitative information about the nature of the processes in the flame. In particular, the study sought to understand the structure of the inhibitor-perturbed flames with regard to temperature and species concentration in the outer region of the flame. Whereas thermocouple measurements can be used in ground based studies, their implementation in drop-tower rigs is limited. A possible approach to determine the temperature field around the flame is to use interferometric techniques. The implementation and testing of a shear-plate interferometry technique is described below. Derived from text

Temperature Measurement; Halogen Compounds; Interferometry; Diffusion Flames; Counterflow; Combustion; Jet Flow; Laminar Flow; Premixing

19970020571 California Univ., Combustion Group, Berkeley. Lawrence Berkeley Lab, CA USA Effects of Buoyancy on Laminar and Turbulent Premixed V-Flame

Cheng, Robert K., California Univ., USA; Bedat, Benoit, California Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 149-153; In English; Also announced as 19970020547

Contract(s)/Grant(s): NASA Order C-32000-R; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Turbulent combustion occurs naturally in almost all combustion systems and involves complex dynamic coupling of chemical and fluid mechanical processes. It is considered as one of the most challenging combustion research problems today. Though buoyancy has little effect on power generating systems operating under high pressures (e.g., IC engines and turbines), flames in atmospheric burners and the operation of small to medium furnaces and boilers are profoundly affected by buoyancy. Changes in burner orientation impacts on their blow-off, flash-back and extinction limits, and their range of operation, burning rate, heat transfer, and emissions. Theoretically, buoyancy is often neglected in turbulent combustion models. Yet the modeling results are routinely compared with experiments of open laboratory flames that are obviously affected by buoyancy. This inconsistency is an obstacle to reconciling experiments and theories. Consequently, a fundamental understanding of the coupling between turbulent flames and buoyancy is significant to both turbulent combustion science and applications. The overall effect of buoyancy relates to the dynamic interaction between the flame and its surrounding, i.e., the so-called elliptical problem. The overall flame shape, its flowfield, stability, and mean and local burning rates are dictated by both upstream and downstream boundary conditions. In steady propagating premixed flames, buoyancy affects the products region downstream of the flame zone. These effects are manifested upstream through the mean and fluctuating pressure fields to influence flame stretch and flame wrinkling. Intuitively, the effects buoyancy should diminish with increasing flow momentum. This is the justification for excluding buoyancy in turbulent combustion models that treats high Reynolds number flows. The objectives of our experimental research program is to elucidate flame-buoyancy coupling processes in laminar and turbulent premixed flames, and to characterize microgravity (micro g) premixed flames. The results are used to derive appropriate scaling parameters for guiding the development of theoretical models to include the effects of buoyancy. Knowledge gain from the analysis will also contribute to further understanding of the elliptical nature of premixed flames. Our current emphasis is to examine the momentum limit above which the effects of buoyancy would become insignificant. This is accomplished by comparing the flowfields and the mean properties of normal gravity flames (+g), and reversed gravity flames (-g, up-side-down flames) at different flow velocities and turbulence intensities. Microgravity (micro g) flames experiments provide the key reference data to reconcile the differences between flames in +g and -g. As flame configuration has significant impact on premixed flames characteristics we have studied axi-symmetric conical flames and plane-symmetric rod-stabilized v-flames. The two configurations produce distinct features that dictates how the flames couple with buoyancy. In a conical flame, the hot products plume completely envelopes the flame cone and shields the flame from direct interaction with the ambient air. The plume originates at the burner rim and generates a divergent flowfield. In comparison, the products region of v-flames forms between the twin flame sheets and it is convergent towards the center-plane. Interaction with ambient air is limited to the two end regions of the stabilized rod and beyond the flame sheets.

Derived from text

Laminar Flow; Microgravity; Flame Propagation; Buoyancy; Premixed Flames; Turbulent Combustion; Combustion Physics

# 19970020573 Naval Research Lab., Lab. for Computational Physics and Fluid Dynamics, Washington, DC USA Unsteady Multidimensional Simulations of the Structure and Dynamics of Flames

Kailasanath, K., Naval Research Lab., USA; Patnaik, G., Naval Research Lab., USA; Oran, E. S., Naval Research Lab., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 161-166; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The primary objective of our research is to develop an understanding of the differences in the structure, stability, dynamics and extinction of flames in earth gravity and in microgravity environments. Numerical simulations, in which the various physical and chemical processes can be independently controlled, can significantly advance our understanding of these differences. Therefore, our approach is to use detailed time-dependent, multidimensional, multispecies numerical models to perform carefully designed computational experiments. Some of these computational experiments are also complementary to physical experiments performed under the Microgravity Combustion Science Program. In this report, we provide a brief summary of our research since the last microgravity combustion workshop. The two major projects we have been working on are: (1) the development and application of a three-dimensional, time-dependent flame model, and (2) a study of the effects of gravity on flame-vortex interactions. A state-of-the-art parallel flame code, FLAME3D, has been developed and used to simulate the three-dimensional cellular structure of lean hydrogen flames. The results from the simulations have been compared to our previous two-dimensional simulations to understand the role of three-dimensionality. This is discussed below in some detail after a brief discussion of the flame code. The second project deals with flame-vortex interactions under different gravitational environments such as zero, upward

and downward Earth gravity. These numerical experiments are complementary to the physical experiments of Driscoll et al reported elsewhere in these proceedings.

Derived from text

Flame Propagation; Microgravity; Vortices; Mathematical Models; Combustion; Gravitational Effects; Simulation; Three Dimensional Models; Time Dependence

# 26 METALLIC MATERIALS

Includes physical, chemical, and mechanical properties of metals, e.g., corrosion; and metallurgy.

19970019302 Los Alamos National Lab., NM USA

Mechanical Response and Microcrack Formation in a Fine-Grained Duplex TiAl at Different Strain Rates and Temperatures

Jin, Zhe, Los Alamos National Lab., USA; Cady, Carl, Los Alamos National Lab., USA; Gray, George T. III, Los Alamos National Lab., USA; Kim, Young-Won, Universal Energy Systems, Inc., USA; 1996; 11p; In English; TMS: Materials Week, 6-10 Oct. 1996. Cincinnati, OH, USA

Contract(s)/Grant(s): W-7405-eng-36

Report No.(s): LA-UR-96-3075; CONF-961017-8; DE96-014931; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

Compressive behavior of this alloy was studied at strain rates of 0.001 sec(exp -1) and 2000 sec(exp -1) and temperatures from -196 C to 1200 C. Temperature dependence of yield stress was found to depend on strain rate: At the quasi-static strain rate, 0.001 sec(sup -1), the yield stress decreases with temperature with a plateau between 200 and 800 C. At the high strain rate, 2000 sec(sup -1), the yield stress exhibits a positive temperature dependence above 600 C. Strain hardening rate decreases dramatically with temperature in the very low and high temperature regions with a plateau at intermediate temperatures for both strain rates. As the strain rate increases, the strain hardening rate plateaus extended to higher temperatures. The strain rate sensitivity increases slightly with temperature (but less than 0.1) for strain rates above 0.001 sec(sup -1). However, at a strain rate of 0.001 sec(sup -1), there is a dramatic increase in the strain rate sensitivity with temperature; above 1100 C, the rate sensitivity becomes much larger. Microcracks occurring in grain interiors and at grain boundaries were observed at all strain rates and temperatures. Formation and distribution of microcracks were found to vary depending on strain rate and deformation temperature.

Microcracks; Titanium Alloys; Yield Strength; Strain Hardening; Strain Rate; Temperature Dependence; Aluminum Alloys

19970019319 Argonne National Lab., Materials Science Lab., IL USA

Spin-density-wave antiferromagnetism of Cr in Fe/Cr(001) superlattices

Fullerton, Eric E., Argonne National Lab., USA; Bader, S. D., Argonne National Lab., USA; Robertson, J. L., Oak Ridge National Lab., USA; [1996]; 15p; In English; 5th; Physics of Transition Metals, 24-27 Sep. 1996, Osaka, Japan Contract(s)/Grant(s): W-31-109-eng-38

Report No.(s): ANL/MSD/CP-90555; CONF-9609168-3; DE96-015088; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The antiferromagnetic Spin-Density-Wave (SDW) order of Cr layers in Fe/Cr(001) superlattices was investigated by neutron scattering. For Cr thickness 51-190 A, a transverse SDW is formed for all temperatures below Neel temperature with a single wavevector Q normal to the layers. A coherent magnetic structure forms with the nodes of the SDW near the Fe-Cr interfaces. For thinner Cr layers, the magnetic scattering can be described by commensurate antiferromagnetic order. DOE

Antiferromagnetism; Chromium Compounds; Iron Compounds; Magnetic Field Configurations

19970019326 California Univ., dept. of Chemical and Biochemical Engineering and Materials Science, Irvine, CA USA Fatigue Mechanisms in Metallic Matrix Composites *Final Report, 1 Jul. 1995 - 30 Jun. 1996* 

Earthman, James C., California Univ., USA; Lavernia, Enrique J., California Univ., USA; Aug. 1996; 13p; In English Contract(s)/Grant(s): F49620-92-J-0262

Report No.(s): AD-A319912; AFOSR-TR-97-0026; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Fatigue crack growth in alumina particulate reinforced Ni3Al alloy composites, IC-50/Al2O3, fabricated using a spray deposition and co-injection process was examined and compared with that in a conventional nickel-based superalloy, Inconel 718.

Single edge-notched fatigue crack growth specimens were tested under constant dK conditions using a custom fully automated servo-hydraulic test system. The results indicate that the threshold value of dK is at least as high as that for monolithic IC-5O, regardless of whether the composite is in the as-sprayed or HIPed condition. However, the HIPed microstructure exhibits a higher fatigue crack growth resistance in the Paris law regime compared to the as-sprayed material. Both composites exhibit a lower crack growth resistance compared to that for unreinforced IC-5O. Compared with Inconel 718, the present IC-5O Metal Matrix Composites (MMCs) consistently exhibit substantially better fatigue crack growth resistance properties.

Metal Matrix Composites; Crack Propagation; Aluminum Alloys; Fatigue Life

## 19970019383 Rockwell International Corp., Thousand Oaks, CA USA

Environmental Integrity of the Coating Metal Interface - Novel Non-VOC Technology *Annual Report*, 1 Oct. 1995 - 30 Sep. 1996

Kendig, Martin W., Rockwell International Corp., USA; Sep 1996; 5p; In English

Contract(s)/Grant(s): N00014-92-C-0215

Report No.(s): AD-A317351; No Copyright; Avail: CASI; A01, Hardcopy; A01, microfiche

Environmental concerns demand a reduction if not total elimination of the emissions of Volatile Organic Compounds (VOCs) from all manufacturing processes. This study seeks to identify the critical factors which will lead to the optimization of a non-VOC epoxy coating and ultimately to produce a prototype non-VOC marine primer. Our goal is to develop an ambient temperature curable epoxy coating that is fully compatible with supercritical CO2 (SOF CO2) without VOC and can meet the performance requirements at least equivalent to Mil Spec 24441. Our efforts have been focused on: (1) studying the relationship between the structure of amine curing agent and its reactivity with SOF CO2 and (2) identifying an amine curing agent that can reversibly release CO2 at a rate fast enough to allow the formation of a coating that is uniform and void free. Our approach entails the deposition of the epoxy resin from a supercritical CO2 (SOF CO2) solution.

DTIC
Organic Compounds; Epoxy Resins; Metal Coatings; Environment Protection

19970019399 Oak Ridge National Lab., TN USA

## Charge-density wave and magnetic phase diagram of chromium alloys

Fishman, R.S., Oak Ridge National Lab., USA; Jiang, X.W., North Dakota State Univ., USA; Aug. 08, 1996; 14p; In English; Magnetism and Magnetic Materials '96, 12 - 15 Nov. 1996, Atlanta, GA, USA

Contract(s)/Grant(s): DE-AC05-96OR-22464

Report No.(s): CONF-961141-4; DE96-015046; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

The magnetic phase diagrams of all dilute Cr alloys can be explained by a simple theoretical model with coupled spin- and charge-density waves and a finite electron reservoir. If the charge-density wave and electron reservoir are sufficiently large, the paramagnetic to commensurate spin-density wave transition becomes strongly first order, as found in Cr(1-x)Fe(x) and Cr(1-x)Si(x) alloys. The observed discontinuity of the slope  $dT(sub\ N)/dx$  at the triple point and the bending of the CI phase boundary are also natural consequences of this model.

DOE

Chromium Alloys; Phase Diagrams; Magnetic Properties; Electric Charge

# 19970019524 Iowa Univ., Dept. of Mechanical Engineering, Iowa City, IA USA

Transport Phenomena During Equiaxed Solidification of Alloys Final Report

Beckermann, C., Iowa Univ., USA; deGroh, H. C., III, NASA Lewis Research Center, USA; Apr. 07, 1997; 136p; In English Contract(s)/Grant(s): NCC3-290

Report No.(s): NASA-CR-204066; NAS 1.26:204066; No Copyright; Avail: CASI; A07, Hardcopy; A02, microfiche

Recent progress in modeling of transport phenomena during dendritic alloy solidification is reviewed. Starting from the basic theorems of volume averaging, a general multiphase modeling framework is outlined. This framework allows for the incorporation of a variety of microscale phenomena in the macroscopic transport equations. For the case of diffusion dominated solidification, a simplified set of model equations is examined in detail and validated through comparisons with numerous experimental data for both columnar and equiaxed dendritic growth. This provides a critical assessment of the various model assumptions. Models that include melt flow and solid phase transport are also discussed, although their validation is still at an early stage. Several

numerical results are presented that illustrate some of the profound effects of convective transport on the final compositional and structural characteristics of a solidified part. Important issues that deserve continuing attention are identified.

Solidification; Binary Alloys; Dendritic Crystals; Microstructure; Macroscopic Equations; Models

19970019560 Illinois Inst. of Tech., Metallurgical Engineering and Materials Science, Chicago, IL USA Synthesis, Characterization, and Properties of Nanometer-Sized Intermetallics *Final Report, 1 Jul. 1992 - 31 Jul. 1995* Dollar, Marek, Illinois Inst. of Tech., USA; Choudry, Mahmood S., Illinois Inst. of Tech., USA; Sep. 1995; 81p; In English Contract(s)/Grant(s): F49620-92-J-0252

Report No.(s): AD-A320458; AFOSR-TR-97-0034; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

Nanocrystalline intermetallics were produced from pre-cast NiAl using electron beam inert gas condensation system. A liquid nitrogen cooled cold finger was used to collect the powder. After collection, the powder was transported under high vacuum to a compaction unit where in-situ compaction at 1.4 Gpa was carried out under vacuum conditions at temperatures ranging from 100 to 300 C. Energy dispersive spectroscopy and X-ray diffraction (XRD) techniques were used to investigate chemical composition, phase and grain size. Average grain size in the range of 2 to 10 nm was found for various specimens. XRD spectra of as consolidated specimens suggested a majority of ordered phase with little disordering in n-NiAl.

Intermetallics; Grain Size; Chemical Composition; Phase Transformations

#### 19970019563 Lawrence Livermore National Lab., Livermore, CA USA

# Electronic structure and phase equilibria in ternary substitutional alloys

Traiber, A. J. S., Massachusetts Inst. of Tech., USA; Allen, S. M., Massachusetts Inst. of Tech., USA; Turchi, P. E. A., Lawrence Livermore National Lab., USA; Waterstrat, R. M., National Inst. of Standards and Technology, USA; Apr. 26, 1996; 50p; In English

Contract(s)/Grant(s): W-7405-eng-48

Report No.(s): UCRL-ID-124587; DE96-050511; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

A reliable, consistent scheme to study phase equilibria in ternary substitutional alloys based on the tight-binding approximation is presented. With electronic parameters from linear muffin-tin orbital calculations, the computed density of states and band structures compare well with those from more accurate ab initio calculations. Disordered alloys are studied within the tight-binding coherent-potential approximation extended to alloys; energetics of ordered systems are obtained through effective pair interactions computed with the general perturbation method; and partially ordered alloys are studied with a novel simplification of the molecular coherent-potential approximation combined with the general perturbation method. The formalism is applied to bcc-based Zr-Ru-Pd alloys which are promising candidates for medical implant devices. Using energetics obtained from the above scheme, we apply the cluster- variation method to study phase equilibria for particular pseudo- binary alloys and show that results are consistent with observed behavior of electronic specific heat coefficient with composition for Zr(0.5)(Ru, Pd)(0.5).

Atomic Structure; Ternary Alloys; Phase Transformations; Order-Disorder Transformations; Body Centered Cubic Lattices; Phase Stability (Materials); Palladium Alloys; Ruthenium Alloys; Zirconium Alloys; Perturbation Theory

# 19970019581 Brookhaven National Lab., Upton, NY USA

#### Exchange-Spring Nd-Fe-B alloys: Investigations into reversal mechanisms and their temperature dependence

Lewis, L. H., Brookhaven National Lab., USA; Welch, D. O., Brookhaven National Lab., USA; Panchanathan, V., Magnequench International, Inc., USA; 1996; 15p; In English; Magnetism and Magnetic Materials, 12-15 Nov. 1996, Atlanta, GA, USA Contract(s)/Grant(s): DE-AC02-76CH-00016

Report No.(s): BNL-63415; CONF-961141-2; DE97-000140; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche In order to investigate factors affecting coercivity a series of two-phase Nd2Fe14B-based nanocomposite alloys with different excess iron concentrations were produced by melt-spinning methods. The constituent grain size was estimated by diffraction methods to be in the range of 150 A - 500 A, and room-temperature demagnetization curves verify that the alloys studied exhibit a modest remanence enhancement. Isothermal remanence magnetization (IRM) and dc-demagnetization (DCD) measurements performed at temperatures in the range 275 K less than or equal to T less than or equal to 350 K illustrate that the coercivity and irreversible magnetization develops in a bimodal, incoherent manner from a demagnetized state but upon demagnetization from a saturated state the system evinces collective, exchange-coupled behavior as illustrated by the reversible magnetization M(sub

rev). The temperature dependencies and values of the irreversible susceptibility X(sub irr) (DCD) suggest that a moderating phase with a magnetic anisotropy intermediate to the two constituent main phases may be present in the alloys. DOE

Demagnetization; Neodymium Alloys; Iron Alloys; Coercivity; Magnetization

19970019589 Carnegie-Mellon Univ., Dept. of Materials Science and Engineering, Pittsburgh, PA USA

Low Temperature Chemical Routes to Synthesis and Processing of Titanium Aluminides Intermetallics *Final Report, 15 Dec. 1994 - 14 Apr. 1996* 

Kumta, Prashant N., Carnegie-Mellon Univ., USA; Jun. 14, 1996; 30p; In English

Contract(s)/Grant(s): F49620-95-I-0088

Report No.(s): AD-A320466; AFOSR-TR-97-0052; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The goal of this project was to synthesize gamma-TiAl using low temperature chemical processing techniques. Four different chemical processes based on the electropositive and reducing power of lithium were used to investigate their potential for the synthesis of the aluminides. The reactions conducted in polar solvents resulted in the formation of TiAl along with TiC as a secondary phase. Among the various polar solvents attempted, THF appears to be the most suitable solvent since the carbide phase was very much reduced. It also appears from these preliminary studies that subjecting the precursors to pre-treatment in H2 makes them stable towards oxidation. Washing the preheated powders in water at this stage helps in minimizing and even elimination to a large extent impurity phases which may be related to lithium. The uses of inert solvents were found to be unsuitable due to the formation of insoluble adducts that lead to the generation of the formation of unknown phases in addition to TiC. The presence of TiC as an impurity is related to the coordination of TiCl with the solvent. The process offers promise and future efforts should be concentrated on removal of the solvent molecules coordinated to the metal groups so that single phase gamma-TiAl can be synthesized. At the same time, it is possible that these TiAl-TiC composites may have some potential structural application.

DIIC

Intermetallics; Aluminides; Titanium; Synthesis (Chemistry); Solvents

# 19970019643 NASA Lewis Research Center, Cleveland, OH USA

#### **Corrosion of Mullite by Molten Salts**

Jacobson, Nathan S., NASA Lewis Research Center, USA; Lee, Kang N., NASA Lewis Research Center, USA; Yoshio, Tetsuo, Okayama Univ., Japan; J. Am. Ceram. Soc.; Aug. 1996; Volume 79, No. 8, pp. 2161-2167; In English

Report No.(s): NASA-TM-112759; NAS 1.15:112759; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The interaction of molten salts of different Na2O activities and mullite is examined with furnace and burner tests. The more-acidic molten salts form small amounts of Al2O3; the more-basic molten salts form various Na2O-Al2O3-SiO2 compounds. The results are interpreted using the Na2O-Al2O3-SiO2 ternary phase diagram, and some possible diffusion paths are discussed. The generally higher melting points of Na2O-Al2O3-SiO2 compounds lead to better behavior of mullite in molten salts, as compared to SiO2-protected ceramics such as SiC. Mullite-coated SiC is discussed, and the corrosion behavior is evaluated. Author

Corrosion; Mullites; Molten Salts; Burners; Furnaces; Aluminum Oxides

# 19970020035 Defence Science and Technology Organisation, Ship Structures and Materials Div., Canberra, Australia The Weld Cracking Susceptibility of High Hardness Armour Steel

Alkemade, S. J., Defence Science and Technology Organisation, Australia; Mar. 1996; 25p; In English

Report No.(s): AD-A318815; DSTO-TR-0320; DODA-AR-009-659; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The work detailed in this paper was performed to determine the likelihood of cracking during and after welding of 10 mm thick, high hardness, armour steel plate in conditions of high restraint. All welding was performed using the pulsed gas metal arc welding process in the flat position. High restraint conditions were tested using the Y-groove test. Welds were performed with ferritic, austenitic and duplex austenitic /ferritic electrodes. Underbead cracking, a typical form of hydrogen induced cracking, was observed in the hardened region of the heat affected zone of ferritic welds where the heat input was 0.5 kJ/mm and the preheat was 750 C or less. No cracking was observed at this heat input when the preheat was raised to 1500 C. When the heat input was raised to 1.2 kJ/mm, no cracking was observed, even when preheat was not used. Underbead cracking was not observed in either austenitic or duplex welds. However, the duplex welds were found to be susceptible to weld metal solidification cracking when the heat input used was low, 0.5 kJ/mm. These cracks did not occur when the heat input was raised to 1.2 kJ/mm.

DTIC

Arc Welding; Welded Joints; Metal Plates; Austenite

#### 19970020093 NASA Lewis Research Center, Cleveland, OH USA

#### Observations of Static Strain-Aging in Polycrystalline NiAl

Weaver, M. L., Florida Agricultural and Mechanical Univ., USA; Noebe, R. D., NASA Lewis Research Center, USA; Lewandowski, J. J., Case Western Reserve Univ., USA; Oliver, B. F., Tennessee Univ., USA; Kaufman, M. J., Florida Univ., USA; Intermetallics; 1966; ISSN 0966-9795; Volume 4, pp. 533-542; In English

Contract(s)/Grant(s): N0001491-J-1370; NSF DMR-89-8326; NGT3-2958

Report No.(s): NASA-CR-204551; NAS 1.26:204551; Copyright Waived (NASA); Avail: CASI; A02, Hardcopy; A01, microfiche

Static strain-aging has been investigated in eight polycrystalline NiAl alloys. After annealing at 1100 K for 7200 s followed by furnace cooling, high-purity, nitrogen-doped, and titanium-doped alloys exhibited continuous yielding, while conventional-purity and carbon-doped alloys exhibited distinct upper yield points and Luders strains. Either water quenching from 1100 K or prestraining via hydrostatic pressurization suppressed the yield points in the latter alloys, but they could be reintroduced by further annealing treatments. Yield points could be reintroduced more rapidly if the specimens were prestrained uniaxially rather than hydrostatically, owing to the arrangement of dislocations into cell structures during uniaxial deformation. Chemical analysis suggests that the species responsible for strain-aging is interstitial carbon.

Alloys; Polycrystals; Nickel; Yield Point; Carbon; Annealing; Aluminum

#### 19970020320 State Univ. of New York, Stony Brook, NY USA

Investigation into the Susceptibility of Corrosion Resistant Alloys to Biocorrosion Final Report, 1 Oct. 1995 - 30 Sep. 1996

Clayton, Clive R., State Univ. of New York, USA; Sep. 1996; 6p; In English

Contract(s)/Grant(s): N00014-96-I-0059

Report No.(s): AD-A317674; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The influence of sulfate-reducing bacteria (SRB) on the passivity of Mo-bearing (type 317L) and low Mo content (type 304) austenitic stainless steels (55) was investigated by x-ray photoelectron spectroscopy (XPS), microbiological and electrochemical techniques. Samples were exposed to SRB, and then the resulting surfaces were analyzed by XPS, and the corrosion resistance by potentiodynamic polarization in deaerated 0.1 M HCl. In order to further understand their passivity, the SRB-exposed samples were also analyzed by XPS after potentiostatic polarization at a passive potential in the hydrochloric solution.

Corrosion Resistance; Bacteria; Austenitic Stainless Steels; Passivity

#### 19970020324 Pennsylvania State Univ., University Park, PA USA

The Characterization of Microbiologically Influenced Corrosion (MIC) Under Cathodic Protection Conditions *Annual Report*, Oct. 1995 - Oct 1996

Macdonald, Digby D., Pennsylvania State Univ., USA; Unz, Richard, Pennsylvania State Univ., USA; Oct. 1996; 82p; In English Contract(s)/Grant(s): N00014-94-1-0027

Report No.(s): AD-A319382; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

The goal of the present research is to investigate the effectiveness of cathodic protection in preventing, halting, or limiting the microbiologically influenced corrosion (MIC) of carbon steel substrates in seawater. MIC is defined as the corrosion resulting from the interaction of bacteria, especially Sulfate Reducing Bacteria (SRB), and their biological end products with metal surfaces. In order to address this problem, four key issues are being investigated. Firstly, the chemical and electrochemical conditions beneath biofilm must be determined. Secondly, the thermodynamic conditions necessary at the surface of the substrate for cathodic protection to be effective must be known. Thirdly, the process by which SRB colonize and adhere to steel surfaces needs to be examined. Finally, the effectiveness of impressed current cathodic protection techniques on inhibiting corrosion due to the presence of biofilms and tubercles on the carbon steel surface must be investigated.

DTIC

Author

Cathodic Coatings; Corrosion Prevention; Bacteria; Carbon Steels; Metal Surfaces

19970020384 Defence Science and Technology Organisation, Aeronautical and Maritime Research Lab., Melbourne, Australia Strength and Fatigue Life Enhancements of Cracked Metal

Finney, J. M., Defence Science and Technology Organisation, Australia; Niessen, C., Defence Science and Technology Organisation, Australia; Absolom, N., Defence Science and Technology Organisation, Australia; Lemm, K., Defence Science and Technology Organisation, Australia; Oct. 1996; 29p; In English

Report No.(s): DSTO-TR-0434; AR-009-913; Copyright; Avail: Issuing Activity (Defence Science and Technology Organiza-

tion, Melbourne, Australia), Hardcopy, microfiche

Plates with cracks were examined experimentally on 2024 aluminum alloy specimens. Measures to reclaim both the static strength and the fatigue life of these plates also was done. The simple measure of stop drilling the crack tips restored most of the tensile strength of the plate. Cold expanding the resulting holes and inserting interference-fit steel plugs has dramatically increased fatigue resistance. For the same spectrum the fatigue life stresses in the life-enhanced plates needed to be 2.6 times those in the plain cracked plates. This factor remained practically constant in the presence of secondary bending when the average bending-stress/axial-stress ratio was 0.5. The secondary bending reduced the fatigue life by only about 25% for both unenhanced and enhanced specimens. The F-111 aircraft can benefit from these results having obvious application to the lower wing skin cracking. CASI

Fatigue Life; Crack Tips; Metals; Tensile Strength; Stress Ratio

# 19970020408 Academy of Sciences of the Ukraine, Kurdyumov Inst. for Metal Physics, Kiev, Ukraine Metal Physics and Advanced Technologies, Volume 18

Molodkin, V. B., Editor, Academy of Sciences of the Ukraine, Ukraine; Tatarenko, V. A., Editor, Academy of Sciences of the Ukraine, Ukraine; Nov. 1996; ISSN 0204-3580; 84p; In Russian; Copyright; Avail: Issuing Activity (National Academy of Sciences of the Ukraine, 36 Academician Vernadsky Blvd., UA-252680 Kiev-142, Ukraine), Hardcopy, microfiche

Papers address the following topics: Electron density of states and electrical conductivity of disordered alloys, investigation of granular electrodeposited Fe-Cu films, application of Green's function to electron scattering based on dynamical theory of scattering by deformed crystals, and specifics of X-ray diffuse scattering as a result of gamma-phase particles formation in single crystals of nickel-based superalloys.

Derived from text

Electron Density (Concentration); Electrical Resistivity; Electrodeposition; Electron Scattering; Single Crystals; X Ray Scattering; Nickel Alloys; Iron Alloys

## 19970020437 NASA Lewis Research Center, Cleveland, OH USA

# Temperature and Strain-Rate Effects on Low-Cycle Fatigue Behavior of Alloy 800H

Rao, K. Bhanu Sankara, NASA Lewis Research Center, USA; Schiffers, H., Kernforschungsanlage, Germany; Schuster, H., Kernforschungsanlage, Germany; Halford, G. R., NASA Lewis Research Center, USA; Metallurgical and Materials Transactions A.; Feb. 1996; Volume 27A, pp. 255-267; In English

Report No.(s): NASA-TM-112753; NAS 1.15:112753; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The effects of strain rate (4 x 10(exp -6) to 4 x 10(exp -3)/s) and temperature on the Low-Cycle Fatigue (LCF) behavior of alloy 800H have been evaluated in the range 750 C to 950 C. Total axial strain controlled LCF tests were conducted in air at a strain amplitude of +/- 0.30 pct. LCF life decreased with decreasing strain rate and increasing temperature. The cyclic stress response behavior showed a marked variation with temperature and strain rate. The time- and temperature- dependent processes which influence the cyclic stress response and life have been identified and their relative importance assessed. Dynamic strain aging, time-dependent deformation, precipitation of parallel platelets of M(23)C6 on grain boundaries and incoherent ledges of twins, and oxidation were found to operate depending on the test conditions. The largest effect on life was shown by oxidation processes.

Author

Temperature Dependence; Strain Rate; Life (Durability); Fatigue (Materials); Alloys

# 27 NONMETALLIC MATERIALS

Includes physical, chemical, and mechanical properties of plastics, elastomers, lubricants, polymers, textiles, adhesives, and ceramic materials. For composite materials see 24 Composite Materials.

# 19970019358 Mitsubishi Heavy Industries Ltd., Hiroshima, Japan

# Improvement of Drain Erosion Resistance of Steam Turbine Blade by Ceramics Coating

Ebara, Ryuichiro, Mitsubishi Heavy Industries Ltd., Japan; Yamada, Yoshikazu, Mitsubishi Heavy Industries Ltd., Japan; Nakagawa, Yoshikiyo, Mitsubishi Heavy Industries Ltd., Japan; Wada, Tetsuyoshi, Mitsubishi Heavy Industries Ltd., Japan; Osaki, Hiroaki, Mitsubishi Heavy Industries Ltd., Japan; Feb. 1997; 8p; In English

Report No.(s): MTB-202; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

In order to prevent drain erosion of turbine moving blades, we have successfully developed a Cr-TiN multilayered coating instead of the stellite plate soldered on the blade surface. The Cr-TiN coatings have been applied to both domestic and foreign steam turbines since 1987. Recently, the three compressor drive turbines of a major chemical company in the U.S.A. have successfully finished 7.5 years of non-stop operation, and the Cr-TiN coating has been found to be in good condition. This paper reports on the fundamental properties, erosion resistance, and application of Cr-TiN coatings in actual turbines.

Author

Erosion; Steam Turbines; Turbine Blades; Ceramic Coatings; Titanium Nitrides; Chromium

#### 19970019502 Los Alamos National Lab., NM USA

## Simulation of a ceramic impact experiment using the SPHINX smooth particle hydrodynamics code

Mandell, D. A., Los Alamos National Lab., USA; Wingate, C. A., Los Alamos National Lab., USA; Schwalbe, L. A., Los Alamos National Lab., USA; 1996; 10p; In English; 16th; Ballistics, 23-28 Sep. 1996, San Francisco, CA, USA Contract(s)/Grant(s): W-7405-eng-36

Report No.(s): LA-UR-96-1878; CONF-960982-2; DE96-012625; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche We are developing statistically based, brittle-fracture models and are implementing them into hydrocodes that can be used for designing systems with components of ceramics, glass, and/or other brittle materials. Because of the advantages it has simulating fracture, we are working primarily with the smooth particle hydrodynamics code SPHINX. We describe a new brittle fracture model that we have implemented into SPHINX, and we discuss how the model differs from others. to illustrate the code's current capability, we simulate an experiment in which a tungsten rod strikes a target of heavily confined ceramic. Simulations in 3D at relatively coarse resolution yield poor results. However, 2D plane-strain approximations to the test produce crack patterns that are strikingly similar to the data, although the fracture model needs further refinement to match some of the finer details. We conclude with an outline of plans for continuing research and development.

Simulation; Ceramics; Impact; Statistical Analysis; Brittleness; Aluminum Oxides; Fracturing; Mechanical Properties

## 19970019504 MSE, Inc., Butte, MT USA

Pressure-Controlled Atomization Process (PCAP) for Dimensional Restoration of Aviation Parts, Part 1 Final Report, Aug. 1990 - May 1995

Tierney, John C., MSE, Inc., USA; Giovan, Ronald J., MSE, Inc., USA; Lee, Ying-Ming, MSE, Inc., USA; Jul. 1996; 208p; In English

Contract(s)/Grant(s): DE-AC22-88ID-12735; AF Proj. 2103

Report No.(s): AD-A317287; AL/EQ-TR-1995-0029-Pt-1; No Copyright; Avail: Issuing Activity (Defense Technical Information Center (DTIC)), microfiche

The Pressure-Controlled Atomization Process (PCAP) is a new thermal spray process in which a liquid metal is atomized in a supersonic nozzle, which also directs the spray to a suitable substrate. The Spray Casting Project was jointly sponsored by the USA Air Force, Armstrong Laboratory Environics Directorate at Tyndall AFB, and the USA Department of Energy, Office of Technology Development (DOE-OTD) under the U.S. Air Force-DOE Memorandum of Understanding (MOU). The Air Force application uses the Pressure Controlled Atomization Process (PCAP) to thermally spray metallic replacement coatings for electroplated hard chromium. The report presents a history of PCAP as it relates to the development of the process, the development of the hardware to support the process development and the testing that was conducted to understand the process and generate engineering data to support the replacement hard chromium electroplating with PCAP sprayed coatings.

Atomizing; Sprayed Coatings; Supersonic Nozzles; Sprayers; Metal Coatings; Liquid Metals; Electroplating

19970019510 Florida Univ., Dept. of Chemistry, Gainesville, FL USA

Organic and Transition Metal Complex Superconductors and Redox Active Conductive Polymers Final Report

Reynolds, John R., Florida Univ., USA; Oct. 07, 1996; 19p; In English

Contract(s)/Grant(s): F49620-92-J-0509; AF Proj. 2303

Report No.(s): AD-A317222; AFOSR-TR-96-0520; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

We have developed and characterized a broad class of synthetic metals and electroactive polymers. Refer to final technical report for AASERT grant F49620-93-1-0322 for an overview of advances made in transition metal complexes as radical anion components in synthetic metals. We have developed a new family of electrochromic polymers utilizing 3,4-ethylenedioxythiophene as an oxidatively polymerizable moiety. These polymers allow Band Gap Engineering such that the full visible spectrum is attained. These polymers have been incorporated into high contrast, dual polymer electrochromic devices which exhibit a high

degree of switching stability (more than 10,000 switches easily attained). Luminescent polyphenylenes have been synthesized having both polar and ionic functionality. These have been incorporated into blue-emitting EL devices using electrostatic deposition methods. A number of external transitions with industry, Air Force personnel, and academic laboratories are underway researching applications for these polymers in electrochromic and electroluminescent devices, along with possibilities as corrosion protection coatings.

**DTIC** 

Transition Metals; Organic Materials; Oxidation-Reduction Reactions

19970019535 Armstrong Lab., Brooks AFB, TX USA

Technical Evaluation of Moving C-130 Engine Compressor Wash Operations Indoor Washrack, Building 228, Little Rock Air Force Base, Arkansas *Final Report*, 23 - 27 Jan. 1995

Schmidt, Franz J., Armstrong Lab., USA; Hemenway, Doris A., Armstrong Lab., USA; Davis, Robert P., Armstrong Lab., USA; Oct. 1996; 35p; In English

Report No.(s): AD-A317152; AL/OE-TR-1996-0129; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Personnel from the Armstrong Laboratory Water Quality Branch conducted Wastewater Characterization on the wastewater from a C-130 Engine Compressor Wash Ope ration at Little Rock AFB, Arkansas, 23-27 Jan 95. Based on the Cadmium and Nickel Mass Balance Models, the scope of the survey was to compare the models with the actual amount of cadmium and nickel in the engine compressor washwater from the point where the washwater fell from the C-130 aircraft to Little Rock AFB's wastewater discharge point. The combined results of the phased investigation led to our recommendations that the base could conduct compressor washes on up to two or three aircraft per day without pretreatment. We recommended that the base carefully monitor and maintain the oil/water separator at Facility 228 as long as compressor washes would be conducted there, to ensure that non-compliance would not result from cadmium in the separator from past operations being released into the sanitary sewer system in subsequent operations, resulting in a slug of heavy metals that could cause a violation of pretreatment agreement limits. Additionally, we recommended that if compressor washes were to be conducted for a long time period, the base should consider an industrial wastewater pretreatment system for heavy metals generated from the operations.

DTIC

Evaluation; Compressors; Performance Tests; Water Quality; C-130 Aircraft; Engines

19970019562 MSE, Inc., Butte, MT USA

Pressure-Controlled Atomization Process (PCAP) for Dimensional Restoration of Aviation Parts, Part 2 Final Report, Aug. 1990 - May 1995

Tierney, John C., MSE, Inc., USA; Giovan, Ronald J., MSE, Inc., USA; Lee, Ying-Ming, MSE, Inc., USA; Jul. 1996; 158p; In English

Contract(s)/Grant(s): DE-AC22-88ID-12735; AF Proj. 2103

Report No.(s): AD-A317288; AL/EQ-TR-1995-0029-Pt-2; No Copyright; Avail: CASI; A08, Hardcopy; A02, microfiche

The Pressure-controlled Atomization Process (PCAP) is a new thermal spray process in which a metal is atomized in a supersonic nozzle, which also directs the spray to a suitable substrate. The Casting Project was jointly sponsored by the USA Air Force, Armstrong Laboratory Environics Directorate at Tyndall AFB, and the USA Department of Energy, Office of Technology Development (OTD) under the U. S. Air Force - DOE Memorandum of Understanding (MOU). The Air Force application the Pressure Controlled Atomization Process (PCAP) to thermally spray metallic replacement coatings for electroplated hard chromium. The report presents a history of PCAP as it relates to the development of the process, the development of the hardware to support the process development, and the testing that was conducted to understand the process and generate engineering data to support the replacement hard chromium electroplating with PCAP sprayed coating.

DTIC

Pressure; Dimensions; Restoration; Atomizing; Spacecraft Components

19970019671 Centre de Recherches Scientifiques et Techniques de l'Industrie des Fabrications Metalliques, Parc Scientifique de la Cense Rouge, Brussels, Belgium

The Assembly of Thermoplastics by Adhesive Bonding: Process and Control

Lecomte, J., Centre de Recherches Scientifiques et Techniques de l'Industrie des Fabrications Metalliques, Belgium; Bolted/Bonded Joints in Polymeric Composites; Jan. 1997; 8p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A02, Hardcopy; A03, microfiche

Nowadays, the manufacturing techniques include more and more frequently the assembling of different materials, each dedicated to fulfill one or several requirements of the final assembly. Product designers are therefore induced to consider adhesive

bonding of thermoplastic materials, either between themselves or to other materials. Adhesive bonding offers several advantages: weight reduction, better stress distribution in the joint, sealing and insulation. However, this type of assembly, especially when the adherents are thermoplastics, raises many questions about the performances in terms of mechanical resistance, durability, and also about the reliability and the control of the joints. This presentation will consider the four design steps which are of primary importance for the conception of an assembly by adhesive bonding.

Author

Adhesive Bonding; Thermoplastic Resins; Thermoplasticity

#### 19970019676 NASA Lewis Research Center, Cleveland, OH USA

# Probabilistic Evaluation of Bolted Joints in Polymer Matrix Composites

Chamis, C. C., NASA Lewis Research Center, USA; Minnetyan, L., Clarkson Univ., USA; Jan. 1997; 16p; In English; Also announced as 19970019652; Copyright Waived; Avail: CASI; A03, Hardcopy; A03, microfiche

Computational methods are described to probabilistically simulate fracture in bolted composite structures. Progressive fracture is simulated via an innovative approach independent of stress intensity factors and fracture toughness. The effect on structure damage of design variable uncertainties is quantified. The Fast Probability Integrator is used to assess the scatter in the composite structure response before and after damage. Sensitivity of the response to design variables is evaluated. The methods are demonstrated for bolted joint polymer matrix composite panels under end loads. The effects of fabrication process are included in the simulation of damage in the bolted panel. The results show that the most effective way to reduce the end displacement at fracture is to control the load and ply thickness.

Author

Bolted Joints; Composite Structures; Fracture Strength; Stress Intensity Factors; Polymer Matrix Composites

## 19970019705 NASA Lewis Research Center, Cleveland, OH USA

## The Oxidation and Protection of Gamma Titanium Aluminides

Brady, Michael P., NASA Lewis Research Center, USA; Brindley, William J., NASA Lewis Research Center, USA; Smialek, James L., NASA Lewis Research Center, USA; Locci, Ivan E., NASA Lewis Research Center, USA; JOM; Nov. 1996; Volume 48, No. 11, pp. 46-50; In English

Report No.(s): NASA-TM-112484; NAS 1.15:112484; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

The excellent density-specific properties of the gamma class of titanium aluminides make them attractive for intermediate-temperature (600-850 C) aerospace applications. The oxidation and embrittlement resistance of these alloys is superior to that of the alpha(sub 2) and orthorhombic classes of titanium aluminides. However, since gamma alloys form an intermixed Al2O3/TiO2 scale in air rather than the desired continuous Al2O3 scale, oxidation resistance is inadequate at the high end of this temperature range (i.e., greater than 750-800 C). For applications at such temperatures, an oxidation-resistant coating will be needed; however, a major drawback of the oxidation-resistant coatings currently available is severe degradation in fatigue life by the coating. A new class of oxidation-resistant coatings based in the Ti-Al-Cr system offers the potential for improved fatigue life.

Oxidation Resistance; Titanium Alloys; Protective Coatings; Aluminum Alloys; Chromium Alloys

19970019750 Massachusetts Inst. of Tech., Lincoln Lab., Lexington, MA USA

Test Tank Evaluation of A Frequency-Scanning, Microwave Radiometer to Estimate Oil Thickness and Physical Properties Final Report, Sep. 1994 - Feb. 1996

Murphy, T. J., Massachusetts Inst. of Tech., USA; McMahon, O. B., Massachusetts Inst. of Tech., USA; Hover, Gary L., Coast Guard Research and Development Center, USA; Apr. 1996; 559p; In English

Contract(s)/Grant(s): F19628-95-C-0002

Report No.(s): AD-A320082; USCG-D-18-96; No Copyright; Avail: CASI; A24, Hardcopy; A04, microfiche

This report describes the testing of a 26-40 GHz (Ka-band) Frequency Scanning Radiometer (FSR) at OHMSETT (the National Oil Spill Response Test Facility) to evaluate the instrument's ability to detect and measure the thickness of oil films on water. Measurement variables were oil type, oil thickness, and wave conditions. The results indicate that the FSR was able to reliably measure oil thickness under calm conditions and, in some cases, under mild wave conditions. Future hardware development should include (1) a multichannel upgrade to the Ka-band FSR to decrease the data acquisition interval, and (2) the development of a proof-of-concept W-band (75-110 GHz) FSR to measure thinner films. After laboratory testing, these instruments should be

evaluated at OHMSETT. Included in the appendices to this report are all of the radiometric Brightness Temperature (TB) versus measurement frequency plots for the data collected at OHMSETT.

**DTIC** 

Evaluation; Measuring Instruments; Oil Slicks

19970019879 Washington State Univ., Dept. of Physics, Pullman, WA USA

Polymer Fibers for Nonlinear Optics Final Report, 1 May 1993 - 30 Apr. 1996

Kuzyk, Mark G., Washington State Univ., USA; Oct. 01, 1996; 13p; In English

Contract(s)/Grant(s): F49620-93-I-0255; AF Proj. 2303

Report No.(s): AD-A317197; AFOSR-TR-96-0516; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

The goal of our research is to assess the possibility of making an ultrafast all-optical switching device. This require the preliminaries of doing materials processing, materials characterization, and making all-device component structures such as single mode fibers. With these in hand, a demonstration all-optical switching device can be made. Such a device would be the first step towards ultrafast switching systems for the information highway and all-optical computing applications. Our work is motivated by the demonstration of an all-optical switch in a silica optical fiber. While this device displays all essential switching functions, the small materials nonlinearity requires fibers 1 km lengths, resulting in long latency periods. Because we have the ability to make polymer fibers with optical nonlinearities that are three orders of magnitude larger, we can make sub-meter length devices. As an ongoing process, have continually improved the fiber drawing process, have characterized crucial material properties, and have improved on designs of optical switches that take advantage of the polymer fiber's nonlinearity. We have demonstrated the fabrication of fibers with cores that are less than 10 micrometers in diameter, have shown that these can support single mode light-guiding (required for optimum device operation), and that they do not depolarize light: an important property for devices that require polarization preserving fibers. The Sagnac interferometer experiment had been used to measure the switching efficiency in a single mode polymer fiber and a true all-optical switching device has been built and has given evidence of all-optical switching.

Optical Switching; Optical Fibers; Optical Data Processing; Nonlinear Optics; Fabrication; Fiber Optics

19970019924 NASA Lewis Research Center, Cleveland, OH USA

## **Internal Radiation Effects in Zirconia Thermal Barrier Coatings**

Siegel, Robert, NASA Lewis Research Center, USA; Journal of Thermophysics and Heat Transfer; Jun. 09, 1996; Volume 10, No. 4, pp. 707-709; In English

Report No.(s): NASA-TM-112842; NAS 1.15:112842; No Copyright; Avail: CASI; A01, Hardcopy; A01, microfiche

Using thermal barrier coatings on combustor liners, turbine vanes, and rotating blades is important for reducing metal temperatures in current and advanced aircraft engines. Zirconia is a common coating material, and it is partially transparent to thermal radiation. Radiation becomes more significant as temperatures are raised for higher efficiency in advanced engines. Calculations are often made with radiation effects neglected inside the coating. The effect of radiation is illustrated here, where an analytical procedure is provided by using the two-flux method for the radiative contribution. A detailed study was made of ceramic thermal barrier coatings for diesel engines, and a two-flux analysis was developed for radiation in semitransparent multilayer composites. These efforts provide the basis for the present analysis where illustrative solutions are obtained for typical conditions in an aircraft engine. The formulation and solution of the exact spectral radiative transfer equations including large scattering, as is characteristic of zirconia, are rather complicated. The two-flux method is used here to provide a simplified method.

Derived from text

Thermal Control Coatings; Aircraft Engines; Radiative Transfer; Thermal Radiation; Zirconium; Differential Equations; Temperature Distribution; Runge-Kutta Method

19970019966 NASA Goddard Space Flight Center, Greenbelt, MD USA

## Reduction of Calcofluor in Solithane Conformal Coatings of Printed Wiring Boards

Miller, Michael K., NASA Goddard Space Flight Center, USA; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 59-65; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

An investigation on the outgassing of a pigment employed as a fluorescent medium in conformal coatings has been performed. The conformal coatings in question are used to protect printed wiring boards from environmental hazards such as dust and moisture. The pigment is included in the coating at low concentration to allow visual inspection of the conformal coating for flaw detection. Calcofluor, the fluorescent pigment has been found to be a significant outgasser under vacuum conditions and a potential source of contamination to flight hardware. A minimum acceptable concentration of Calcofluor for flaw detection is

desirable. Tests have been carried out using a series of Solithane(TM) conformal coating samples, with progressively lower Calcofluor concentrations, to determine the minimum required concentration of Calcofluor. It was found that the concentration of Calcofluor could be reduced from 0.115% to 0.0135% without significant loss in the ability to detect flaws, while at the same time significant reductions in Calcofluor outgassing and possible contamination of systems could be realized.

Author

Printed Circuits; Pigments; Outgassing; Dust; Defects; Contamination

# 19970019989 California State Univ., Dept. of CIAM, Northridge, CA USA

# Combined Effects of Fluxes of Atomic Oxygen and Electrons on Chemical Reactions with Polymeric Materials

Shively, Jon, California State Univ., USA; King, Thomas, Phillips Lab., USA; Miglionico, Charles, Phillips Lab., USA; Robertson, Robert, Phillips Lab., USA; Davis, Steven, Phillips Lab., USA; Stein, Charles, Phillips Lab., USA; Wilson, Warren, Phillips Lab., USA; Baird, James, Alabama Univ., USA; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 305-314; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Understanding the phenomenology of the interaction of the space environment with organic-composite spacecraft surfaces is both interesting science and important to the longevity of our space assets. The importance of this understanding has been made even more critical by the desire to use new organic composite materials whose lower weight and higher stiffness will make it possible to orbit larger payloads. Inconsistencies between ground simulation and space test data clearly indicate that our understanding of the interaction phenomenology is inadequate. This paper describes the test equipment, designed by Phillips Laboratory, to subject materials to a simulated low-earth-orbit (LEO) environment, consisting of simultaneous fluxes of hyper-thermal neutral oxygen atoms (AO), energetic electrons, vacuum-ultraviolet light, and hypervelocity-particle impacts characteristic of space debris and micrometeoroids. Preliminary results of studies of the combined effects of fluxes of AO and electrons on polysulfone resins and composites are presented. The chemical species generated by chemical reactions were monitored using a mass spectrometer, and the results indicate that the primary effect of electrons on AO reactions is through electric fields induced by charging the material surface.

Author

Oxygen Atoms; Earth Orbital Environments; Low Earth Orbits; Micrometeoroids; Organic Materials; Payloads; Phenomenology; Resins; Stiffness; Spacecraft Construction Materials

# 19970019991 Soreq Research Establishment, Israel Atomic Energy Commission, Yavneh, Israel Oxygen and VUV Irradiation of Polymers: Atomic Force Microscopy (AFM) and Complementary Studies

Grossman, E., Soreq Research Establishment, Israel Atomic Energy Commission, Israel; Noter, Y., Soreq Research Establishment, Israel Atomic Energy Commission, Israel; Lifshitz, Y., Soreq Research Establishment, Israel Atomic Energy Commission, Israel; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 333; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A01, Hardcopy; A04, microfiche; Abstract Only; Abstract Only

Materials in low earth orbit (LEO) are exposed to the various constituents of the space environment, including atomic oxygen (ATOX) and solar UV radiation. While their separate interactions with a variety of materials are frequently well understood, the synergistic interactions are much less so. The present study investigate the effects of oxygen and vacuum UV (VUV) irradiation on two types of polymers commonly used for space applications: fluorocarbons (such as Teflon FEP, Tefzel or Tedlar, having different C/F ratio) and polyimides (Kapton H). As a VUV source we employed a deuterium lamp with a magnesium fluoride window that provided radiation between 115 and 300 nm. The oxygen source was a Kaufman source ion beam. Various fluences of oxygen and VUV were used. The applied radiation schemes were: (1) oxygen, (2) VUV, (3) oxygen followed by VUV, (4) VUV followed by oxygen, and (5) simultaneous oxygen and VUV. Atomic Force Microscopy (AFM) was found to be very powerful in detecting the surface degradation from the very early stage. Very low oxygen or VUV fluxes effects which are not detectable using any other surface sensitive technique were observed by the AFM. Complementary techniques included mass loss measurements, changes in surface composition (by XPS) and analysis of the released gases by Residual Gas Analyzer (RGA). Teflon FEP and Kapton H were found to exhibit different behavior. While Teflon FEP demonstrated VUV sensitivity and an appreciable synergistic effect, Kapton H showed high oxygen reactivity and less significant synergistic effect. These effects will be demonstrated by comparing the results of samples exposed to the different radiation schemes.

Author

Aerospace Environments; Atomic Force Microscopy; Far Ultraviolet Radiation; Photoelectron Spectroscopy; Vacuum Effects; Ultraviolet Radiation; Teflon (Trademark)

#### 19970020026 Los Alamos National Lab., NM USA

# Chelating water-soluble polymers for waste minimization

Smith, B., Los Alamos National Lab., USA; Cournoyer, M., Los Alamos National Lab., USA; Duran, B., Los Alamos National Lab., USA; Ford, D., Los Alamos National Lab., USA; Gibson, R., Los Alamos National Lab., USA; Lin, M., Los Alamos National Lab., USA; Meck, A., N. P. Energy, Inc., USA; Robinson, P., N. P. Energy, Inc., USA; Robison, T., Los Alamos National Lab., USA; [1996]; 13p; In English

Contract(s)/Grant(s): W-7405-eng-36

Report No.(s): LA-UR-96-3224; DE97-000534; No Copyright; Avail: Issuing Activity (Department of Energy (DOE)), microfiche

Within the DOE complex and in industry there is a tremendous need for advanced metal ion recovery and waste minimization techniques. This project sought to employ capabilities for ligand-design and separations chemistry in which one can develop and evaluate water-soluble chelating polymers for recovering actinides and toxic metals from various process streams. Focus of this work was to develop and select a set of water-soluble polymers suitable for a selected waste stream and demonstrate this technology in 2 areas: removal of (a) actinides and toxic RCRA metals from waste water and (b) recovery of Cu and other precious metals from industrial process streams including from solid catalysts and aqueous waste streams. The R&D was done in 4 phases for each of the 2 target areas: polymer synthesis for scaleup, equipment assembly, process demonstration at a DOE or industrial site, and advanced ligand/polymer synthesis. The TA- 50 site at Los Alamos was thought to be appropriate due to logistics and to its being representative of similar problems throughout the DOE complex.

DOE

Polymers; Waste Water; Water Reclamation; Waste Treatment; Actinide Series; Chelation; Metal Ions; Noble Metals; Toxicity

# 19970020054 Department of the Navy, Washington, DC USA

Novel Linear Metallocene Polymers Containing Acetylenic and Inorganic Units and Thermosets and Ceramics Therefrom Keller, Teddy, Inventor, Department of the Navy, USA; Houser, Eric J., Inventor, Department of the Navy, USA; Mar. 14, 1997; 53p; In English

Patent Info.: Filed 14 Mar. 1997; US-Patent-Appl-SN-818193

Report No.(s): AD-D018411; No Copyright; Avail: Issuing Activity (Dept. of the Navy, Washington DC), microfiche

Transition metal containing ceramic or carbonaeous material are formed from novel linear polymers contain ing a random distribution of repeating acetylenic units, organotransition metal complexes, Siloxane, boron, Silicon, and/or carborane-siloxane units. The precursor thermosets are formed by crosslinking of the linear polymers through the acetylenic units in the polymer backbone. The ceramics may also be formed directly by pyrolysis of the linear polymers. The preceramic polymers are potentially useful for fabricating ceramic fibers and composite materials having enhanced strength, hardness and toughness as well as superior mechanical, optical, electrical and/or magnetic properties.

DTIC

Transition Metals; Composite Materials; Linear Systems

19970020062 Army Armament Research, Development and Engineering Center, Benet Labs., Watervliet, NY USA Internal Stresses, Texture, and Anisotropy in High-Contraction Electroplated Chromium Coatings Final Report

Lee, S. L., Army Armament Research, Development and Engineering Center, USA; Capsimalis, G. P., Army Armament Research, Development and Engineering Center, USA; Sep. 1996; 26p; In English

Report No.(s): AD-A319770; ARCCB-TR-96027; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Internal residual stresses in refractory coatings of the bore cause cracking, flaking, peeling, and failure of the coatings and substrate. Strong fiber texture, perfect in-plane azimuthal symmetry, low single-crystal anisotropy, and high-surface tensile residual stresses were observed in high-contraction chromium on steel. The conventional d-square of sin(psi) method fails in the evaluation of residual stress if the existence of texture is not taken into account. Elastic moduli were evaluated from single-crystal elastic constants. Two methods were developed to extract residual stresses in textured chromium coatings: (1) A new matlab matrix inversion method using a single family of reflections. The method allows calculation of residual stress and unstrained lattice parameter in textured cubic materials. (2) A Hill-Neerfeld model assuming elastic isotropy. This is a d-square of sin(psi) method adapted to multiple families of reflections.

**DTIC** 

Residual Stress; Protective Coatings; Stress Analysis

# 19970020088 Clarkson Univ., Dept. of Mechanical and Aeronautical Engineering, Potsdam, NY USA Fabrication of Reticulated Graphitic Foam

Anderson, Heather J., Clarkson Univ., USA; Jan. 09, 1997; 85p; In English

Report No.(s): AD-A320069; AFIT-96-120; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

Carbon foams have applications where light weight and high temperature resistant materials are required. A 3D morphology can be obtained, forming an intricate network of interconnecting struts. These struts have the potential to simulate graphitic carbon fibers with a high specific strength, high specific stiffness, high thermal conductivity, and extreme high temperature stability. Potential applications of carbon foams include: fugitive phase for inverse metal foams, rapid thermal capacitors, catalyst substrates, 3D composite reinforcement, and caustic and biological filters. Carbon foams have been produced using blowing agents such as carbon dioxide and nitrogen, however these foams contain closed cells and have a microcellular morphology. The goal of the present work is to produce a graphitic carbon foam with open cells on the order of 10 to 18 ppi (pores per inch). A technique has been developed using polyurethane foam as a fugitive phase. The polyurethane foam is dipped into a solution of mesophase pitch (MP). Mesophase pitch is a carbon precursor, in the present case, derived from naphthalene. The advantage of MP is that it is easily graphitized. The flow of the MP over the struts gives some initial molecular orientation. The dipped foam is dried, leaving behind a the polyurethane foam coated with the pitch. The foam then goes through several heat treatments to stabilize the mesophase pitch, burn out the polyurethane, carbonize and finally graphitize the foam, all the while maintaining the same morphology as the initial polyurethane foam.

**DTIC** 

Refractory Materials; Foams; Polyurethane Foam; Carbon; Fabrication; Graphitization; Morphology; Thermal Stability; Polyurethane Resins; Thermal Resistance

19970020212 Purdue Univ., School of Aeronautics and Astronautics, West Lafayette, IN USA

Fracture and Fatigue of Piezoelectric Ceramics and Development of an Adaptive Sandwich Structure *Final Report, 1 Aug.* 1992 - 31 May 1996

Sun, C. T., Purdue Univ., USA; Oct. 1996; 89p; In English

Contract(s)/Grant(s): F49620-92-J-0457

Report No.(s): AD-A317561; AF-AFOSR-TR-0537-96; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

Smart materials such as SMA and piezoelectric materials offer promising applications in many adaptive structures enabling the development of new structural control. Potential applications include shape control of large space structures, active noise and vibration control, flutter suppression, and microservoelasticity in flight vehicles. to deliver the maximum actuation power, piezoelectric actuators are subjected to high electric fields and strains. The development of reliability and life prediction methodologies for piezoceramics is of vital importance to the technology of smart structures. The result of this research concerning the behavior of fracture and fatigue crack growth in PZT piezoceramics under combined electrical and mechanical loads is an important step to the aforementioned goal.

DTIC

Fracturing; Fatigue (Materials); Piezoelectric Ceramics; Sandwich Structures; Cermets

19970020282 Naval Surface Warfare Center, Carderock Div., Bethesda, MD USA

## An Evaluation of Low Energy Cure Glass Fabric Prepregs

Juska, Thomas, Naval Surface Warfare Center, USA; Loup, Doug, Naval Surface Warfare Center, USA; Mayes, Steven, Naval Surface Warfare Center, USA; Sep. 1996; 57p; In English

Report No.(s): AD-A317523; NSWCCD-TR-65-96/23; No Copyright; Avail: CASI; A04, Hardcopy; A01, microfiche

Low energy cure glass fabric prepregs were evaluated. These materials were formulated to cure at low temperatures, from 140 F to 220 F, and under vacuum bag pressure. Several of these material systems are now commercially available and have potential applications in high quality, low cost fabrication of surface ship structures. Most of the prepreg resins are epoxy, but polyester and vinyl ester laminates were included in the evaluation. The test laminates were fabricated with a warps parallel lay-up and tested in tension, compression, flexure, and impact. Limited in-plane shear testing was done, particularly to assess the advantage of a quasi-isotropic vs. warps parallel stacking sequence. Thermal analysis was used to determine as-fabricated, post-cured, and moisture conditioned values of Tg. Single-sided prepreg and no-tack prepreg were identified as useful material forms for achieving low void content under vacuum bag pressure. The low cure temperature of the prepregs allows vacuum bag fabrication of sandwich panels with a variety of foam cores.

**DTIC** 

Fabrication; Glass; Thermal Analysis; Sandwich Structures; Prepregs; Laminates; Epoxy Compounds

19970020289 Naval Surface Warfare Center, Carderock Div., Bethesda, MD USA

# Use of Enzymatic Cleaners on U.S. Navy Ships Topical Report

Venkatachalam, R. S., Naval Surface Warfare Center, USA; Mar. 1996; 90p; In English

Report No.(s): AD-A317420; NSWCCRD-TR-63-CR-96/09; NSWCCARDIV-TR-96/002; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

The Naval Surface Warfare Center, Carderock Division, conducted a study to determine the feasibility of using enzymatic and bacterial products in cleaning applications aboard U.S. Navy ships. A review of the most recent technical literature and a survey of potential suppliers were conducted. In addition, shipboard systems, subsystems and housekeeping processes were evaluated to identify suitable applications for enzymatic and bacterial cleaners. The study identified numerous commercial products that, based on manufacturers' claims, would be effective and safe for use aboard ship to clean walls, floors, galley work surfaces, engine and machine parts, drains, pipes, grease traps, Collection, Holding and Transfer (CHT) tanks, ballast tanks and bilge areas. However, the study also revealed the absence of standardized test protocols essential for validation of manufacturers' claims, and recommended the cooperative development of such protocols by representatives from the commercial sector, Government and academia. The need to obtain meaningful cost information based on actual use scenarios and to investigate any permitting issues associated with the discharge of related wastes to pierside facilities was also identified.

Feasibility; Enzyme Activity; Cleaners; Ships; Bacteria

19970020399 Department of the Navy, Washington, DC USA

# A Two Phase HfB2-SiB4 Material

Wuchina, Eric J., Inventor, Department of the Navy, USA; Jun. 24, 1996; 15p; In English

Patent Info.: Filed 24 Jun. 1996; US-Patent-Appl-SN-669673

Report No.(s): NASA-TM-112844; NAS 1.15:112844; No Copyright; Avail: Issuing Activity (Defense Technical Information Center (DTIC)), microfiche

A two phase HfB2-SiB4 material which is useful as a high temperature oxidation resistant coating. This invention relates to ceramic coatings and more particularly to ceramic coatings containing metal borides. Boride materials are known to have good oxidation resistance, with HfB2 considered to be the best pure boride for oxidation applications. It has been shown that the addition of 10 to 20 percent SiC to HfB2 increases the oxidation resistance. The HfB2-SiC materials are prepared by hot pressing powder mixtures. Hot pressing powder mixtures has limited ability to produce fine grained multiphase materials due to particle coarsening during the sintering process. Additionally, the purity of the final monolithic structure is limited to the purity of the starting powders. Chemical vapor deposition (CVD) offers a method of producing highly pure multiphase ceramics, with better control of microstructure. Researchers have tried to produce HfB2-SiC coatings by CVD but without success.

DTIC

**DTIC** 

Ceramic Coatings; Oxidation Resistance; Vapor Deposition; Oxidation; Silicon Compounds; Hot Pressing; Coating; Borides; Powder (Particles)

19970020428 Department of the Navy, Washington, DC USA

#### Phase Stabilization of Zirconia

Provenzano, Virgil, Inventor, Department of the Navy, USA; Holtz, Ronald L., Inventor, Department of the Navy, USA; Lewis, David, Inventor, Department of the Navy, USA; Jan. 30, 1997; 13p; In English

Patent Info.: Filed 30 Jan. 1997; US-Patent-Appl-SN-791292

Report No.(s): AD-D018400; No Copyright; Avail: Issuing Activity (Dept. of the Navy, Washington, DC), microfiche

Stabilized zirconia containing sintered particles of alumina and zirconia in tetragonal phase is prepared by mixing alumina particles of less than 30 nanometers with zirconia particles of less than 30 nanometers in, presence of a liquid to form a suspension, drying the suspension at a temperature up to about 600 C to remove the liquid and products thereof to form a dried suspension composed of agglomerated alumina and zirconia particles, sintering the dried suspension to fuse the particles and cooling the sintered dried suspension to an ambient temperature to produce free-standing bodies or coatings on substrates.

**DTIC** 

Aluminum Oxides; Zirconium Oxides; Sintering; Phase Stability (Materials); Synthesis (Chemistry)

# 28 PROPELLANTS AND FUELS

Includes rocket propellants, igniters, and oxidizers; their storage and handling procedures; and aircraft fuels. For related information see also 07 Aircraft Propulsion and Power, 20 Spacecraft Propulsion and Power, and 44 Energy Production and Conversion.

19970019607 Armstrong Lab., Tyndall AFB, FL USA

JP-8 Composition and Variability Final Report, Aug. 1994 - Feb. 1995

Mayfield, Howard T., Armstrong Lab., USA; May 1996; 35p; In English

Report No.(s): AD-A317177; AL/EQ-TR-1996-0006; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

This report is intended to provide information on the chemical composition of JP-8 fuel for use in assessing the impact of this fuel's use. The composition information contained in this report was obtained from a snapshot sampling of JP-8 fuel in use worldwide. Although it was not possible to obtain samples from all JP-8 locations, the samples obtained from regional aerospace fuels laboratories in Italy, Tampa, FL., Dayton, OH, and Mukilteo, WA are expected to include coverage of most worldwide suppliers of this type of fuel. The fuel samples were analyzed by gas chromatography/mass spectrometry using a medium high resolution gas chromatographic separation. A large number of the hydrocarbon components in the samples were identified and quantitated using a target compound analysis scheme which combined gas chromatographic and mass spectral information in an effort to ensure the correct compounds were quantitated and that in terferences from co-eluting compounds were minimized. In addition to this careful attempt at quantifying most of the hydrocarbon constituents of the fuel, the raw chromatographic peak areas of the total ion chromatograms were examined, and the components responsible for the 100 peaks with the largest average areas were tentatively identified from the mass spectral data.

**DTIC** 

JP-8 Jet Fuel; Chemical Composition; Elution; Fuels; Hydrocarbon Fuels; Hydrocarbons

19970019620 United Technologies Research Center, East Hartford, CT USA

Theoretical Research Investigation of High Energy Species Final Report, 3 May 1990 - 1 Oct. 1996

Michels, H. H., United Technologies Research Center, USA; Nov. 1996; 80p; In English

Contract(s)/Grant(s): F04611-90-C-0009; AF Proj. 5730

Report No.(s): AD-A319054; PL-TR96-3025; No Copyright; Avail: CASI; A05, Hardcopy; A01, microfiche

A theoretical investigation was conducted of high energy chemical species that are attractive candidates for advanced propulsion systems. The objectives of this research program were to identify those light element molecular species that have sufficient internal energy to be useful in advanced chemical propulsion systems; to characterize their molecular structure, energy content and structural or radiative stability; to examine the probable kinetic routes for decomposition of these species; to characterize the vibrational and electronic spectra and other static molecular properties; and to propose possible synthesis routes for their formation and subsequent storage. Experimental data collected at other laboratory sites where there were parallel studies of high energy chemical species - specifically, SRI International, Rockwell Science Center, Rocketdyne, and Phillips Laboratory - were iteratively examined and integrated with the results generated by this theoretical investigation. A goal of this theoretical investigation was to furnish fundamental data and to provide a better understanding of the possibilities of forming chemical compounds that represent advanced high energy sources. It was also intended that this theoretical research effort be carried out with sufficient flexibility to aid in the analysis and guidance of any concurrent experimental programs of synthesis of high energy molecular species. to this end, the tanks of this research program to date have included the following studies: (1) high symmetry and hypervalent structures as advanced oxidizers; (2) azide-like species such as N7 and NO2N3; (3) nitrated cyclic and polycyclic compounds, as further developments of cyclic nitramines such as the HMX and PCN family of propellants; and (4) an extensive analysis of dinitramide compounds as potential chlorine-free oxidizers

**DTIC** 

Cyclic Compounds; Hydrazines; Molecular Structure; Synthesis (Chemistry); High Energy Propellants; Chemical Propulsion; HMX

19970020376 Prins Maurits Lab. TNO, Rijswijk, Netherlands

Temperature and strain gauge measurements in the TNO-PML Cook-off test Final Report

Scholtes, J. H. G., Prins Maurits Lab. TNO, Netherlands; vanderMeer, B. J., Prins Maurits Lab. TNO, Netherlands; Jan. 1997; 35p; In English; Originl contains color illustrations

Contract(s)/Grant(s): A95/KL/408

Report No.(s): TD96-0039; TNO-PML-1996-A62; Copyright; Avail: Issuing Activity (Prins Maurits Lab., TNO, The Hague, Netherlands), Hardcopy, microfiche

During the years of development, many modifications were made to the test object. In this configuration, test data can be obtained to verify the thermal/chemical Cook-off computer models. Because the general interest is more focused on the level of severity in a Cook-off event, the development of the TNO-PML Cook-off test went in the same direction. Detonation and Deflagration to Detonation Transition (DDT) experiments have been carried out to measure the strain/strain rate during the last phase of the explosion. The results show a trend in the increasing rate of strain of the different phases of the DDT experiment. First results of the Cook-off experiments look very promising, although a quantitative analyses is not yet possible. The radial temperature distribution curves in the centre of the Cook-off experiments reveal interesting information about endothermic and exothermic reaction steps, and melting and crystal phase transitions of the explosive substances.

Temperature Distribution; Temperature Measurement; Strain Gages; Detonation

19970020407 Prins Maurits Lab. TNO, Rijswijk, Netherlands

Evaluation of the Friability test Final Report Evaluatie van de Friability test

Scholtes, J. H. G., Prins Maurits Lab. TNO, Netherlands; vanderMeer, B. J., Prins Maurits Lab. TNO, Netherlands; Jan. 1997; 25p; In Dutch; Original contains color illustrations

Contract(s)/Grant(s): A94/KL/408

Author (revised)

Report No.(s): TD96-0036; TNO-PML-1996-A59; Copyright; Avail: Issuing Activity (Prins Maurits Lab., TNO, Rijswijk, Netherlands), Hardcopy, microfiche

The test is applied to determine the effect of impact on an explosive substance which is a candidate to be assigned as an Extremely Insensitive Detonating Substance (EIDS). In this test a sample is directed against a steel plate with a velocity of about 150 m/s with the use of a gas gun. After having performed this test, the explosive is tested in the 'closed vessel' test to assess any changes in the burning characteristic, i.e. the peak pressure and pressure rise rate, due to the impact. The volume of the existing 'closed vessel' needed to be adjusted in order to fulfill the calibration requirements with respect to weak pressure (80 +/- 0.2 MPa) and pressure rise rate (not more than 15.2 +/- MPa/msec). This calibration was performed using a reference propellant delivered by SNPE. It appears that both calibration requirements could not be met by the 'closed vessel'. he requirement for the peak pressure could be fulfilled, but not for the pressure rise rate. Nine experiments were satisfactorily performed using the friability test. of two explosives, a standard rocket propellant and a PBX-HMX propellant, the burning characteristics were determined with the 'closed vessel' test. Both propellants broke into numerous pieces in the friability test. Nevertheless the results obtained from the 'closed vessel' test show that both the peak pressure and the pressure rise rate are moderate compared to the reference propellant. Author (revised)

Explosives; Rocket Propellants; Sensitivity; Gas Guns; Combustion; Detonation

# 29 MATERIALS PROCESSING

Includes space-based development of products and processes for commercial applications. For biological materials see 55 Space Biology.

19970019344 Georgia Inst. of Tech., George W. Woodruff School of Mechanical Engineering, Atlanta, GA USA Non-Coalescence Effects in Microgravity Interim Report, 17 Jun. 1996 - 16 Jun. 1997

Neitzel, G. Paul, Georgia Inst. of Tech., USA; May 1997; 44p; In English

Contract(s)/Grant(s): NAG3-1894

Report No.(s): NASA-CR-204492; NAS 1.26:204492; No Copyright; Avail: CASI; A03, Hardcopy; A01, microfiche

Non-coalescence of two bodies of the same liquid and the suppression of contact between liquid drops and solid surfaces is being studied through a pair of parallel investigations being conducted at the Georgia Institute of Technology and the Microgravity Research and Support (MARS) Center in Naples, Italy. Both non-coalescence and contact suppression are achieved by exploiting the mechanism of thermocapillary convection to drive a lubricating film of surrounding gas (air) into the space between the two liquid free surfaces (non-coalescence) or between the drop free surface and the solid (contact suppression). Experiments performed to date include flow visualization experiments in both axisymmetric and (nearly) two-dimensional geometries and quantitative measurements of film thickness in the contact-suppression case in both geometries.

Author

Liquid Surfaces; Solid Surfaces; Microgravity; Flow Visualization; Film Thickness; Drops (Liquids); Liquid-Solid Interfaces; Liquid-Liquid Interfaces

## 19970019899 NASA Marshall Space Flight Center, Huntsville, AL USA

# Advancement of X-Ray Microscopy Technology and its Application to Metal Solidification Studies

Kaukler, William F., Alabama Univ., USA; Curreri, Peter A., NASA Marshall Space Flight Center, USA; SPIE Proceedings Series; Aug. 05, 1996; Volume 2809, pp. 33-44; In English; Space Processing of Materials, 4-5 Aug. 1996, Denver, CO, USA

Report No.(s): NASA-CR-204618; NAS 1.26:204618; ISBN-0-8194-2197; Copyright Waived (NASA); Avail: CASI; A03, Hardcopy; A01, microfiche

The technique of x-ray projection microscopy is being used to view, in real time, the structures and dynamics of the solid-liquid interface during solidification. by employing a hard x-ray source with sub-micron dimensions, resolutions of 2 micrometers can be obtained with magnifications of over 800 X. Specimen growth conditions need to be optimized and the best imaging technologies applied to maintain x-ray image resolution, contrast and sensitivity. It turns out that no single imaging technology offers the best solution and traditional methods like radiographic film cannot be used due to specimen motion (solidification). In addition, a special furnace design is required to permit controlled growth conditions and still offer maximum resolution and image contrast.

Author

X Ray Sources; Microscopy; X Rays; Imaging Techniques; Radiography; Image Contrast

#### 19970019982 CSA Engineering, Inc., Palo Alto, CA USA

# Simulation of the Zero-Gravity Environment for Dynamic Testing of Structures

Kienholz, David A., CSA Engineering, Inc., USA; Nineteenth Space Simulation Conference Cost Effective Testing for the 21st Century; Jan. 1997, pp. 219-230; In English; Also announced as 19970019961; No Copyright; Avail: CASI; A03, Hardcopy; A04, microfiche

Simulation of unconstrained (free-free) boundary conditions is a longstanding problem in ground vibration testing of space-craft. The test article weight must be supported without introducing constraining forces due to stiffness, inertia, or friction from the suspension system. High-fidelity simulation of the space environment requires that such constraint forces be kept small compared to forces inherent in the experiment. A multipoint, six degree of freedom suspension system for dynamic testing is described. Intended primarily for highly flexible space structures, it uses a combination of passive pneumatic and active electromagnetic subsystems. The suspension offers a wide payload range, near-zero stiffness, zero static deflection, small added mass, and zero friction. The electromagnetic system can also provide active cancellation of added mass, accurate ride-height control, and integrated disturbance input. Several versions of the system are described, aimed at test articles ranging from very flexible solar arrays to a 7000-lb simulated optical truss. The concept and hardware are described, test results are given, and applications experience from several industry, government, and university installations is discussed.

Author

Aerospace Environments; Vibration; Large Space Structures; Payloads; Solar Arrays; Degrees of Freedom; Flexible Spacecraft; Trusses; Space Environment Simulation

## 19970020276 NASA Marshall Space Flight Center, Huntsville, AL USA

# Directional Solidification of Mercury Cadmium Telluride During the Second USA Microgravity Payload Mission (USMP-2)

Gillies, D. C., NASA Marshall Space Flight Center, USA; Lehoczky, S. L., NASA Marshall Space Flight Center, USA; Szofran, F. R., NASA Marshall Space Flight Center, USA; Watring, D. A., NASA Marshall Space Flight Center, USA; Alexander, H. A., NASA Marshall Space Flight Center, USA; Jerman, G. A., NASA Marshall Space Flight Center, USA; SPIE Proceedings Series; Aug. 05, 1996; Volume 2809, pp. 1-11; In English; Space Processing of Materials, 4-5 Aug. 1996, Denver, CO, USA Report No.(s): NASA-CR-204619; NAS 1.26:204619; ISBN-0-8194-2197; Copyright Waived (NASA); Avail: CASI; A02, Hardcopy; A01, microfiche

As a solid solution semiconductor having, a large separation between liquidus and solidus, mercury cadmium telluride (MCT) presents a formidable challenge to crystal growers desiring an alloy of high compositional uniformity. To avoid constitutional supercooling during Bridgman crystal growth it is necessary to solidify slowly in a high temperature gradient region. The necessary translation rate of less than 1 mm/hr results in a situation where fluid flow induced by gravity on earth is a significant factor in material transport. The Advanced Automated Directional Solidification Furnace (AADSF) is equipped to provide the stable thermal environment with a high gradient, and the required slow translation rate needed. Ground based experiments in AADSF show clearly the dominance of flow driven transport. The first flight of AADSF in low gravity on USMP-2 provided an opportunity to test theories of fluid flow in MCT and showed several solidification regimes which are very different from those observed

on earth. Residual acceleration vectors in the orbiter during the mission were measured by the Orbital Acceleration Research Experiment (OARE), and correlated well with observed compositional differences in the samples.

Author

Mercury Cadmium Tellurides; Directional Solidification (Crystals); Crystal Growth; Solidus; Liquidus; Temperature Gradients; Bridgman Method

## 19970020317 Universities Space Research Association, Huntsville, AL USA

# Development of Uniform Microstructures in Immiscible Alloys by Processing in a Low-Gravity Environment

Grugel, R. N., Universities Space Research Association, USA; Brush, L. N., Washington Univ., USA; SPIE Proceedings Series; Aug. 05, 1996; Volume 2809, pp. 257-262; In English; Space Processing of Materials, 4-5 Aug. 1996, Denver, CO, USA Contract(s)/Grant(s): NAGw-4301

Report No.(s): NASA-CR-204616; NAS 1.26:204616; ISBN-0-8194-2197; No Copyright; Avail: CASI; A02, Hardcopy; A01, microfiche

Highly segregated macrostructures tend to develop during processing of hypermonotectic alloys because of the density difference existing between the two liquid phases. The approximately 4.6 seconds of low-gravity provided by Marshall Space Flight Center's 105 meter drop tube was utilized to minimize density-driven separation and promote uniform microstructures in hypermonotectic Ag-Ni and Ag-Mn alloys. For the Ag-Ni alloys a numerical model was developed to track heat flow and solidification of the bi-metal drop configuration. Results, potential applications, and future work are presented.

Author

Microstructure; Silver Alloys; Magnesium Alloys; Nickel Alloys; Liquid Phases; Microgravity

# 19970020547 NASA Lewis Research Center, Cleveland, OH USA

# **Fourth International Microgravity Combustion Workshop**

Sacksteder, Kurt R., Compiler, NASA Lewis Research Center, USA; May 1997; 542p; In English; 4th, 19-21 May 1997, Cleveland, OH, USA; Sponsored by NASA Washington, USA; Also announced as 19970020548 through 19970020631; Original contains color illustrations

Contract(s)/Grant(s): RTOP 963-80-0J

Report No.(s): NASA-CP-10194; E-10678; NAS 1.55:10194; No Copyright; Avail: CASI; A23, Hardcopy; A04, microfiche

This Conference Publication contains 84 papers presented at the Fourth International Microgravity Combustion Workshop held in Cleveland, Ohio, from May 19 to 21, 1997. The purpose of the workshop was twofold: to exchange information about the progress and promise of combustion science in microgravity and to provide a forum to discuss which areas in microgravity combustion science need to be expanded profitably and which should be included in upcoming NASA Research Announcements (NRA).

Author

Conferences; Microgravity; Combustion; Flames

## 19970020548 NASA Washington, Washington, DC USA

#### **NASA Microgravity Combustion Science Program**

King, Merrill K., NASA Washington, USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 3-10; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Combustion is a key element of many critical technologies used by contemporary society. For example, electric power production, home heating, surface and air transportation, space propulsion, and materials synthesis all utilize combustion as a source of energy. Yet, although combustion technology is vital to our standard of living, it poses great challenges to maintaining a habitable environment. For example, pollutants, atmospheric change and global warming, unwanted fires and explosions, and the incineration of hazardous wastes are major problem areas which would benefit from improved understanding of combustion. Effects of gravitational forces impede combustion studies more than most other areas of science since combustion involves production of high-temperature gases whose low density results in buoyant motion, vastly complicating the execution and interpretation of experiments. Effects of buoyancy are so ubiquitous that their enormous negative impact on the rational development of combustion science is generally not recognized. Buoyant motion also triggers the onset of turbulence, yielding complicating unsteady effects. Finally, gravity forces cause particles and drops to settle, inhibiting deconvoluted studies of heterogeneous flames important to furnace, incineration and power generation technologies. Thus, effects of buoyancy have seriously limited our capabilities to carry out 'clean' experiments needed for fundamental understanding of flame phenomena. Combustion scientists can use microgravity to simplify the study of many combustion processes, allowing fresh insights into important problems via a deeper un-

derstanding of elemental phenomena also found in Earth-based combustion processes and to additionally provide valuable information concerning how fires behave in microgravity and how fire safety on spacecraft can be enhanced.

Author

Combustion; Propulsion; Microgravity; Flames; Gravitational Effects; Environment Effects; Combustion Physics; NASA Programs

## 19970020550 Northwestern Univ., Evanston, IL USA

#### **Gravitational Effects in Smoldering and SHS**

Matkowsky, Bernard J., Northwestern Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 19-24; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Smolder waves and SHS (self-propagating high-temperature synthesis) waves are both examples of filtration combustion waves propagating in porous media. Smoldering combustion is important for the study of fire safety. Smoldering itself can cause damage, its products are toxic and it can also lead to the more dangerous gas phase combustion which corresponds to faster propagation at higher temperatures. In SHS, a porous solid sample, consisting of a finely ground powder mixture of reactants, is ignited at one end. A high temperature thermal wave, having a frontal structure, then propagates through the sample converting reactants to products. The SHS technology appears to enjoy a number of advantages over the conventional technology, in which the sample is placed in a furnace and 'baked' until it is 'well done'. The advantages include shorter synthesis times, greater economy, in that the internal energy of the reactions is employed rather than the costly external energy of the furnace, purer products, simpler equipment and no intrinsic limitation on the size of the sample to be synthesized, as exists in the conventional technology.

Derived from text

Gravitational Effects; Combustion; Flame Propagation; Combustion Chemistry; Self Propagation; Filtration; Heat of Combustion; Chemical Reactions

# 19970020551 Colorado School of Mines, Dept. of Metallurgical and Materials Engineering, Golden, CO USA The Effect of Gravity on the Combustion Synthesis of Porous Ceramics and Metal Matrix Composites

Moore, J. J., Colorado School of Mines, USA; Woodger, T. C., Colorado School of Mines, USA; Wolanski, T., Colorado School of Mines, USA; Yi, H. C., Guigne International Ltd., Canada; Guigne, J. Y., Guigne International Ltd., Canada; Fourth International Microgravity Combustion Workshop; May 1997, pp. 25-30; In English; Also announced as 19970020547 Contract(s)/Grant(s): CSA-4700468-1; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

Combustion synthesis (self propagating, high temperature synthesis-SHS) is a novel technique that is capable of producing many advanced materials. The ignition temperature (Tig) of such combustion synthesis reactions is often coincident with that of the lowest melting point reactant. The resultant liquid metal wets and spreads around the other solid reactant particles of higher melting points, thereby improving the reactant contact and kinetics, followed by formation of the required compounds. This ignition initiates a combustion propagating wave whose narrow reaction front rapidly travels through the reactants. Since this process is highly exothermic, the heat released by combustion often melts the reactant particles ahead of the combustion front and ignites the adjacent reactant layer, resulting in a self-sustaining reaction. Whenever a fluid phase (liquid or gas) is generated by the reaction system, gravity-driven phenomena can occur. Such phenomena include convective flows of fluid by conventional or unstable convection and settling of the higher density phases. A combustion process is often associated with various kinds of fluid flow. For instance, if the SHS reaction is carried out under inert or reactive gas atmospheres, or a volatile, e.g., B2O3, is deliberately introduced as a reactant, convective flows of the gas will occur due to a temperature gradient existing in the atmosphere when a combustion wave is initiated. The increased gas flow will produce a porous (or expanded) SHS product. Owing to the highly exothermic nature of many SHS reactions, liquid phase(s) can also form before, at, or after the combustion front. The huge temperature gradient at the combustion front can induce convective flows (conventional or unstable) of the liquid phase. Each of these types of convective fluid flow can change the combustion behavior of the synthesizing reaction, and, therefore, the resultant product microstructure. In addition, when two or more phases of different density are produced at or ahead of the propagating combustion front settling of the higher density phase will occur resulting in a non-uniform product microstructure and properties. Derived from text

Combustion Synthesis; Ceramics; Metal Matrix Composites; Flame Propagation; Exothermic Reactions; Convective Flow; Gravitational Effects; Ignition Temperature; Reaction Kinetics

19970020552 Notre Dame Univ., Dept. of Chemical Engineering, IN USA

The Effects of Gravity on Combustion and Structure Formation During Combustion Synthesis in Gasless Systems
Varma, Arvind, Notre Dame Univ., USA; Mukasyan, Alexander, Notre Dame Univ., USA; Pelekh, Aleksey, Notre Dame Univ., USA;
Fourth International Microgravity Combustion Workshop; May 1997, pp. 31-36; In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1644; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

There have been relatively few publications examining the role of gravity during combustion synthesis (CS), mostly involving thermite systems. The main goal of this research was to study the influence of gravity on the combustion characteristics of heterogeneous gasless systems. In addition, some aspects of microstructure formation processes which occur during gasless CS were also studied. Four directions for experimental investigation have been explored: (1) the influence of gravity force on the characteristic features of heterogeneous combustion wave propagation (average velocity, instantaneous velocities, shape of combustion front); (2) the combustion of highly porous mixtures (with porosity greater than that for loose powders), which cannot be obtained in normal gravity; (3) the effect of gravity on sample expansion during combustion, in order to produce highly porous materials under microgravity conditions; and (4) the effect of gravity on the structure formation mechanism during the combustion synthesis of poreless composite materials.

Derived from text

Combustion Synthesis; Flame Propagation; Gravitational Effects; Porous Materials; Microgravity; Microstructure

# 19970020554 Colorado Univ., Mechanical Engineering Dept., Boulder, CO USA

# The Effect of Gravity on the Combustion of Bulk Metals

Branch, Melvyn C., Colorado Univ., USA; Abbud-Madrid, Angel, Colorado Univ., USA; Daily, John W., Colorado Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 43-48; In English; Also announced as 19970020547; Original contains color illustrations

Contract(s)/Grant(s): NAG3-1685; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

In recent years, metal combustion studies at the University of Colorado have focused on the effects of gravity (g) on the ignition and burning behavior of bulk metals. The impetus behind this effort is the understanding of the ignition conditions and flammability properties of structural metals found in oxygen (O2) systems for space applications. Since spacecraft are subjected to higher-than-1g loads during launch and reentry and to a zero-gravity environment while in orbit, the study of ignition and combustion of bulk metals at different gravitational accelerations is of great practical concern. From the scientific standpoint, studies conducted under low gravity conditions provide simplified boundary conditions, since buoyancy is removed, and make possible the identification of fundamental ignition and combustion mechanisms. This investigation is intended to provide experimental verification of the influence of natural convection on the burning behavior of metals. In addition, the study offers the first findings of the influence of gravity on ignition of bulk metals and on the combustion mechanism and structure of metal-oxygen, vapor-phase diffusion flames in a buoyancy-free environment. Titanium (Ti) and magnesium (Mg) metals were chosen because of their importance as elements of structural materials and their simple chemical composition-pure metals instead of multicomponent alloys to simplify chemical and spectroscopic analyses. In addition, these elements present the two different combustion modes observed in metals: heterogeneous or surface burning (for Ti) and homogeneous or gas-phase reaction (for Mg). Finally, Mg, Ti, and their oxides exhibit a wide range of thermophysical and chemical properties. Metal surface temperature profiles, critical and ignition temperatures, propagation rates, burning times, and spectroscopic measurements are obtained under normal and reduced gravity. Visual evidence of all phenomena is provided by high-speed photography.

Derived from text

Metal Combustion; Gravitational Effects; Chemical Analysis; Metals; Titanium; Vapor Phases; Magnesium; Combustion Chemistry; Metal Surfaces

## 19970020557 Michigan Univ., Ann Arbor, MI USA

# Radiation Temperature and Extinction of Transient Gaseous Diffusion Flames in Microgravity

Atreya, Arvind, Michigan Univ., USA; Everest, David A., Michigan Univ., USA; Agrawal, Sanjay, Michigan Univ., USA; Anderson, Michael K., Michigan Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 63-68; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The absence of buoyancy-induced flows in micro g and the resulting increase in the reactant residence time significantly alters the fundamentals of many combustion processes. Substantial differences between 1-g and micro g flames have been reported in experiments on candle flames, flame spread over solids, droplet combustion and others. These differences are more basic than just in the visible flame shape. Longer residence times and higher concentration of combustion products in the flame one create a thermochemical environment which changes the flame chemistry and the heat and mass transfer processes. Processes such as flame radiation (and its interaction with flame chemistry), that are often ignored under normal gravity, become very important and sometimes even controlling. This is particularly true for conditions at extinction of a micro g diffusion flame. The lack of buoyant flow in micro g also enhances the flame radiation due to: (1) build-up of combustion products in the flame zone which increases the gas radiation, and (2) longer residence times make conditions appropriate for substantial amounts of soot to form which is usually responsible for most of the radiative heat loss. Thus, it is anticipated that radiative heat loss may eventually extin-

guish the already 'weak' micro g diffusion flame. While this is a convincing hypothesis, space shuttle experiments on candle flames show that in an infinite ambient atmosphere, the hemispherical candle flame in micro g will burn indefinitely. It is hoped that radiative extinction can be experimentally shown by the aerodynamically stabilized gaseous diffusion flames for certain conditions. Identifying these conditions (ambient atmosphere, fuel flow rate, fuel type, fuel additives, etc.) is important for spacecraft fire safety. The objective of this research is to experimentally and theoretically investigate the radiation-induced extinction of gaseous diffusion flames and understand the interaction of flame radiation with flame chemistry.

Derived from text

Microgravity; Combustion Physics; Flames; Gaseous Diffusion; Fuel Flow; Extinction; Buoyancy; Drops (Liquids); Radiant Cooling; Combustion Products; Flame Propagation

# 19970020558 Princeton Univ., Dept. of Mechanical and Aerospace Engineering, NJ USA Studies of Flame Structure in Microgravity

Law, C. K., Princeton Univ., USA; Sung, C. J., Princeton Univ., USA; Zhu, D. L., Princeton Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 69-74; In English; Also announced as 19970020547; Original contains color illustrations

Contract(s)/Grant(s): NAG3-1713; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

The present research endeavor is concerned with gaining fundamental understanding of the configuration, structure, and dynamics of laminar premixed and diffusion flames under conditions of negligible effects of gravity. Of particular interest is the potential to establish and hence study the properties of spherically- and cylindrically-symmetric flames and their response to external forces not related to gravity. For example, in an earlier experimental study of the burner-stabilized cylindrical premixed flames, the possibility of flame stabilization through flow divergence was established, while the resulting one-dimensional, adiabatic, stretchless flame also allowed an accurate means of determining the laminar flame speeds of combustible mixtures. We have recently extended our studies of the flame structure in microgravity along the following directions: (1) Analysis of the dynamics of spherical premixed flames; (2) Analysis of the spreading of cylindrical diffusion flames; (3) Experimental observation of an interesting dual luminous zone structure of a steady-state, microbuoyancy, spherical diffusion flame of air burning in a hydrogen/methane mixture environment, and its subsequent quantification through computational simulation with detailed chemistry and transport; (4) Experimental quantification of the unsteady growth of a spherical diffusion flame; and (5) Computational simulation of stretched, diffusionally-imbalanced premixed flames near and beyond the conventional limits of flammability, and the substantiation of the concept of extended limits of flammability. Motivation and results of these investigations are individually discussed.

Derived from text

Gravitational Effects; Premixed Flames; Diffusion Flames; Laminar Flow; Microgravity; Fuel Combustion

# 19970020567 Yale Univ., Dept. of Mechanical Engineering, New Haven, CT USA

## Computational and Experimental Study of Laminar Diffusion Flames in a Microgravity Environment

Long, Marshall, Yale Univ., USA; Walsh, Kevin, Yale Univ., USA; Smooke, Mitchell, Yale Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 123-128; In English; Also announced as 19970020547; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

A detailed computational and experimental study of coflow diffusion flames in a microgravity environment has been initiated. The overall goal of the program is to apply adaptive computational algorithms and advanced imaging techniques to a simple, well-characterized burner. The results will provide new information on the formation of NO(x), soot, and the interaction of convection, diffusion, and chemistry in a nonbuoyant environment. In previous work on this flame at normal gravity, quantitative two-dimensional species concentration profiles were modeled computationally and were measured using spontaneous Raman scattering and laser-induced fluorescence (LIF). In extending the study to microgravity conditions, improvements to the computational model have been made and new calculations performed for a range of gravity conditions. In addition, modifications to the experimental approach have been necessitated by the constraints imposed by existing microgravity facilities. Initial results from the computations and experiments are presented in the following sections.

Derived from text

Laminar Flow; Algorithms; Burners; Diffusion Flames; Microgravity; Imaging Techniques; Combustion Chemistry

# 19970020572 Georgia Inst. of Tech., School of Aerospace Engineering, Atlanta, GA USA

# **Turbulent Premixed Flame Propagation in Microgravity**

Menon, S., Georgia Inst. of Tech., USA; Disseau, M., Georgia Inst. of Tech., USA; Chakravarthy, V. K., Georgia Inst. of Tech., USA; Jagoda, J., Georgia Inst. of Tech., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 155-160;

In English; Also announced as 19970020547

Contract(s)/Grant(s): NAG3-1610; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

A facility in which turbulent Couette flow could be generated in a microgravity environment was designed and built. to fit into the NASA Lewis drop tower the device had to be very compact. This means that edge effects and flow re-circulation were expected to affect the flow. The flow was thoroughly investigated using LDV and was found to be largely two dimensional away from the edges with constant turbulence intensities in the core. Slight flow asymmetries are introduced by the non symmetric re-circulation of the fluid outside the test region. Belt flutter problems were remedied by adding a pair of guide plates to the belt. In general, the flow field was found to be quite similar to previously investigated Couette flows. However, turbulence levels and associated shear stresses were higher. This is probably due to the confined re-circulation zone reintroducing turbulence into the test section. An estimate of the length scales in the flow showed that the measurements were able to resolve nearly all the length scales of interest. Using a new LES method for subgrid combustion it has been demonstrated that the new procedure is computational feasible even on workstation type environment. It is found that this model is capable of capturing the propagation of the premixed names by resolving the flame in the LES grid within 2-3 grid points. In contrast, conventional LES results in numerical smearing of the flame and completely inaccurate estimate of the turbulent propagation speed. Preliminary study suggests that there is observable effect of buoyancy in the 1g environment suggesting the need for microgravity experiments of the upcoming experimental combustion studies. With the cold flow properties characterized, an identical hot flow facility is under construction. It is assumed that the turbulence properties ahead of the flame in this new device will closely match the results obtained here. This is required since the hot facility will not enable LDV measurements. The reacting flow facility is also being constructed with planned drop tower experiments in mind. Therefore, issues related to safety and structural integrity are being take into account. Further development of the numerical model will also be carried out to include finite-rate kinetics for representative premixed cases. More detail analysis of the flame structure and propagation nature will be investigated. Simulations will also be compared to the flame properties observed in the experiments.

Derived from text

Premixed Flames; Microgravity; Flame Propagation; Couette Flow; Turbulent Flow; Turbulent Combustion; Reacting Flow; Simulation

# 19970020574 Michigan Univ., Dept. of Aerospace Engineering, Ann Arbor, MI USA

**Premixed Flame-Vortex Interactions Imaged in Microgravity** 

Driscoll, J. F., Michigan Univ., USA; Sichel, M., Michigan Univ., USA; Sinibaldi, J. O., Michigan Univ., USA; Fourth International Microgravity Combustion Workshop; May 1997, pp. 167-172; In English; Also announced as 19970020547 Contract(s)/Grant(s): NAG3-1639; No Copyright; Avail: CASI; A02, Hardcopy; A04, microfiche

A unique experiment makes it now possible to obtain detailed images in microgravity showing how an individual vortex causes the wrinkling, stretching, area increase, and eventual extinction of a premixed flame. The repeatable, controllable flame-vortex interaction represents the fundamental building block of turbulent combustion concepts. New information is provided that is central to turbulent flame models, including measurements of all components of flame stretch, strain, and vorticity. Simultaneous measurements of all components of these quantities are not possible in fully turbulent flames but are possible in the present axisymmetric, repeatable experiment. Advanced PIV diagnostics have been used at one-g and have been developed for microgravity. Numerical simulations of the interaction are being performed at NRL. It is found that microgravity conditions greatly augment the flame wrinkling process. Flame area and the amplitude of wrinkles at zero-g are typically twice that observed at one-g. It is inferred that turbulent flames in microgravity could have larger surface area and thus propagate significantly faster than those in one-g, which is a potential safety hazard. A new mechanism is identified by PIV images that shows how buoyancy retards flame wrinkling at one-g; buoyancy produces new vorticity (due to baroclinic torques) that oppose the wrinkling and the stretch imposed by the original vortex. Microgravity conditions remove this stabilizing mechanism and the amplitude of flame wrinkling typically is found to double. Microgravity also increases the flame speed by a factor of 1.8 to 2.2. Both methane and propane-air flames were studied at the NASA Lewis drop tower. Results indicate that it is important to add buoyancy to models of turbulent flames to simulate the correct flame wrinkling, stretch and burning velocity. Derived from text

Premixed Flames; Vortices; Turbulent Combustion; Particle Image Velocimetry; Microgravity; Flame Propagation; Buoyancy

# 31 ENGINEERING (GENERAL)

Includes vacuum technology; control engineering; display engineering; cryogenics; and fire prevention.

19970019346 NASA Langley Research Center, Hampton, VA USA

**Experimental Robot Position Sensor Fault Tolerance Using Accelerometers and Joint Torque Sensors**